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Thermal Conductivity of Gases. III. Some Values of the Thermal Conductivities of Argon, Helium, and Nitrogen from 0 °C to 75 °C at Pressures of 1×10^5 to 2.5×10^7 Pascals*

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(November 8, 1974)

Accurate measurements of the thermal conductivities of Ar and He agree with the theoretical value of 2.5 $\phi\eta c_v$ (η = viscosity, c_v = specific heat capacity at constant volume ϕ is a number slightly greater than 1 depending upon the intermolecular potential). Measurements of the thermal conductivities of N_2 at 9.6 and 75 °C as a function of pressure up to 2.53×10^7 Pa help to appraise the validity of other measurements of the thermal conductivities of dense gases. The excess conductivity of nitrogen (the additional conductivity resulting from pressure) is shown to be a function of only the density of the nitrogen from 0 to 700 °C and pressures up to 1.3×10^8 Pa.
Key words: Excess thermal conductivity of N_2; thermal conductivity of Ar; thermal conductivity of He; thermal conductivity of N_2.

1. Introduction

The values of thermal conductivities being reported in this paper were obtained by the author at the Massachusetts Institute of Technology. They were to have been part of a more extensive set of measurements, but further work was not completed with this equipment because the author came to the National Bureau of Standards. Even though the number of these results is small, the measurements are thought to be sufficiently accurate to be useful in three respects:

(1) Some measurements of the thermal conductivities of helium allow the factor $f = K/(\eta c_v)$ to be more exactly evaluated. It had appeared to be anomalously low. In this equation K is the thermal conductivity, η the viscosity, and c_v the specific heat capacity at constant volume.

(2) Some measurements of the thermal conductivities of argon, in combination with the values for helium, provide high and low values for calibration of other devices for relative determinations of the thermal conductivities of gases.

(3) Some measurements of the thermal conductivities of nitrogen, up to 2.53×10^7 Pa of pressure, help to provide a guide for evaluating the accuracy of other determinations of the thermal conductivities of dense gases.

2. Experimental Procedure

Measurements were made on the equipment and by the procedures described in previous publications [1, 2].[1] Briefly, the "thermal conductivity cell" was a concentric cylinder type, used with its axis vertical. It was made of silver, and consisted of an "emitter," "guard," "receiver," and "receiver extension." The emitter was a cylinder about 2.2 cm in diameter and 11.4 cm long. It was surrounded by the receiver except at its upper end, and was held in place by spacing pins so that a uniform "conductivity gap" of 0.068 cm was attained. The guard and receiver extension comprised an extension of the emitter and receiver at the upper end of the cell and extended the cell geometry adjacent to them.

The power input was determined by potentiometric measurements of the emf's across two voltage dividers, one to evaluate the potential drop across the heater and the other to evaluate the potential drop across a standard resistor. The temperature difference between the emitter and the receiver was determined from the measured emf's of two Chromel–P Alumel difference couples, one pair of junctions near the top and one pair about midway of the length of the emitter.

Electrical power was supplied to the emitter heater, usually in such amounts as to produce differential thermocouple emf's of 50, 100, and 2[illegible] μV. However, whenever the temperature rise was so large that turbulent convection was detected, the measurements were made with less power. For helium, the available power was only sufficient to heat the emitter to a temperature that produced an emf of 50 μV on the difference thermocouples.

The observed quantities were the ambient temperature, measured by a calibrated platinum resistance

*This work was performed at the Massachusetts Institute of Technology and sponsored by project SQUID, which was supported by the Office of Naval Research, Department of the Navy, under Contract Nonr 1858(25) NR–098–038. Reproduction in full or in part is permitted for use of the United States Government.

[1] Figures in brackets indicate the literature references at the end of this paper.

thermometer, the pressure measured by a deadweight gage and emf's, as follows: (1) a value of the emf of a voltage divider for a standard resistor, V_{std}, (2) a value of the emf of a voltage divider for the emitter heater, V_{em}, (3) a value of the emf of the upper emitter-receiver Chromel–P Alumel difference couple and (4) a value of the emf of the middle emitter-receiver Chromel–P Alumel difference couple $\Delta V_{\Delta t}$. The two difference couple readings were averaged to give $\Delta V_{\overline{\Delta t}}$, and the "apparent conductivity" observed is then

$$K = q/(C\Delta t) = (V_{std} V_{em}/\Delta V_{\overline{\Delta t}}) \times (D\, dE/dt) = \psi\,(D\, dE/dt). \quad (1)$$

The quantity D is a product of calibration constants and the thermal expansion of silver and dE/dt is the thermoelectric power of the thermocouples. In general for each level of power input, two groups of emf's were measured, each group consisting of three complete sets. The temperature of the bath was adjusted according to the power input so that the average gas temperature in the conductivity gap was constant. The values of the ratio $\psi = V_{std} \times V_{em}/\Delta V_{\overline{\Delta t}}$, plotted versus the average thermocouple emf's, $(\Delta V_{\overline{\Delta t}})$, were extrapolated so the intercept, ψ_0, represented a ratio free of heat transfer by convection [1].

2.1. Argon

Argon gas was introduced into the cell directly from a tank of "lamp grade" gas (stated to be more than 99.99% pure). The six sets of emf's at a power level sufficient to produce about a 200 μV thermocouple emf are presented in the following table as a typical example:

TABLE 1. *Sample data for* $Ar_{(a)}$ *at 0 °C and* 1×10^5 *Pa pressure*

Emitter–receiver					
(1)	(2)	(3)	(4)		
V_{std} (μV)	V_{em} (μV)	Upper $\Delta V_{\Delta t}$ (μV)	Middle $\Delta V_{\Delta t}$ (μV)	Average $\Delta V_{\overline{\Delta t}}$ (μV)	ψ (μV)
3467.2	4217.9	197.19	197.61	197.40	7.4085
3460.6	4209.8	196.17	196.32	196.25	7.4236
3458.3	4206.1	195.85	195.98	195.92	7.4244
3502.6	4261.6	200.44	200.66	200.55	7.4430
3503.2	4262.3	200.60	200.87	200.73	7.4387
3503.3	4262.4	200.74	200.99	200.87	7.4339

The comparison of ψ for Ar at 0 °C at each power level showed no dependence on temperature rise (i.e., no detectable transfer of heat by convection), so that ψ_0 was obtained by averaging the results.

$$10^{-4}\psi_0 = 1/3(7.4285 + 7.4247 + 7.4340) = 7.4291\ \mu V$$

with an estimate of the standard deviation of ± 0.15 percent.

The extrapolated values of ψ for argon at 25 °C and 1 atm pressure were obtained from the equation

$$\psi = \psi_0 + A\ \Delta V_{\overline{\Delta t}}$$

with the following values of constants resulting from a least squares solution:

$$\psi_0 = 7.78717 \times 10^4\ \mu V$$

$$A = 23.96.$$

The estimate of the standard deviation from the straight line is $S = 70\ \mu$V.

2.2. Helium

Helium gas, stated to be more than 99.99 percent pure, was used directly from the tank. The measurements of helium were carried out with one-fourth the temperature rises used for Ar, and showed no significant dependence on the size of the temperature gradient. The thermal conductivity of helium was measured in four states: At 2.39×10^5 Pa and 0.00 °C, at 1.01×10^7 Pa and 0.00 °C, at 2.39×10^5 Pa and 75 °C, and at 1.01×10^7 Pa and 75 °C. The measurements at 2.39×10^5 Pa pressure and average gas temperature of 75.00 °C gave clear evidence of progressive contamination of the helium by desorption from the apparatus, and it never became possible to repeat them. Hence there are only three valid values of ψ_0. It was expected that the absolute uncertainty in the emitter-receiver difference couples remained the same for all measurements, and was of marginal significance for the usual range. However, the temperature rise possible was only one-fourth that used for Ar and N_2, and so the higher $\Delta V_{\Delta t}$ values should have the higher relative accuracy. The averages were therefore weighted according to the temperature rise.

At 2.39×10^5 Pa pressure and 0.00 °C,

$$10^{-5}\psi_0 = 1/7\{4\ (6.30376) + 2\ (6.30357) + 6.28868\} = 6.30151$$

with an estimate of the standard deviation of 0.15 percent.

At 1.01×10^7 Pa pressure and 0.00 °C,

$$10^{-5}\psi_0 = 1/7\{4\ (6.48407) + 2\ (6.48556) + 6.52213\} = 6.48993$$

with an estimate of the standard deviation of 0.15 percent.

At 1.01×10^7 Pa pressure and 75.00 °C,

$$10^{-5}\psi_0 = 1/7\{4\ (7.28658) + 2\ (7.28520) + 7.25989\} = 7.28794$$

with an estimate of the standard deviation of 0.15 percent.

2.3 Nitrogen

Nitrogen gas was introduced from the tank directly into the thermal conductivity apparatus. The thermal conductivities of nitrogen gas were determined for 1×10^5 and $1.01=10^7$ Pa pressure at 9.60 °C, and for 1×10^5, 1.01×10^7 and 2.53×10^7 Pa pressure at 75 °C. The temperature rise of the emitter was large enough to produce emf's of the difference thermocouples as large as 200 μV (about 5 °C), and some dependence on temperature rise was observed at all pressures. The extrapolated values of χ were calculated by the method of least squares for the equation

$$\psi=\psi_0+A\ \Delta V_{\overline{\Delta t}}$$

with the following results:

TABLE 2. *Constants for nitrogen equation by least-squares determination*

t	10^5 Pa	ψ_0	A	S
9.60	1	109,567	2.5775	159
9.60	101	134,307	13.452	99
75.00	1	126,009	0.5888	119
75.00	101	143,527	6.9634	61
75.00	253	176,387	18.983	182

The quantity S is the estimate of the standard deviation from the straight line.

The thermal conductivities were determined by calculations, first of "apparent thermal conductivities," and then of "net conductivities." The apparent conductivity is given by eq (1) where

$$D=X/(C_{23}\cdot\phi(t)\cdot R_{std})=5.534_7\times10^{-9}/\phi\ (t)\ \text{w m}^{-1}\text{K}^{-1},$$

with X the product of the voltage divider factors, C_{23} the cell constant at 23 °C and R_{std} the value of the standard resistance. The relative thermal expansion of silver is

$$\phi(t)=1/l_{23}\ \Delta l/\Delta t$$

$$=1+0.1862\times10^{-4}\ (t-23\ ^\circ\text{C})+7.4\times10^{-9}\ (t-23\ ^\circ\text{C})^2.$$

The thermoelectric power, dE/dt, is the calibrated emf for the Chromel–P Alumel thermocouples in μV/K, and has been reported previously [2].

The net or true conductivity is $K=K_{app}-K_{vac}+\Sigma\delta K$, where K_{vac} accounts for the power transferred in a vacuum and $\Sigma\delta K$ consists of 3 relatively small corrections:

(1) fK_{app}, to account for the assymetric temperature distribution of the emitter.

(2) $-7\times10^{-4}\ K_{app}$, to account for the change of heat flow through the pins with increasing conductivity of the medium in the conduction gap.

(3) 0.02556 $(K_{app})^2$, to account for the temperature differences arising in the metal body of the cell between the thermocouple junctions and the conduction gap, for both the emitter and the receiver.

The values of the factors and the net conductivities are given in table 3.

TABLE 3. *Summary of thermal conductivity calculations* K *in units of w* m^{-1} K^{-1}

t °C	10^5 P (Pa)	ψ_0 (μV)	10^9 D	dE/dt	10^2 K_{app}	10^2 K_{vac}	f	$0.02556\times K_{app}$	$\frac{\Sigma\delta K}{K_{app}}$	10^2 K	kgρ/m^3
Argon											
0.00	1.01	74291	5.537	41.51	1.707_4	0.0578	0.0010	0.0004	0.0007	1.651	1.78
25.00	1.01	77872	5.535	42.43	1.828_7	.0645	.0010	.0004	.0007	1.765	1.64
Helium											
0.00	2.39	630151	5.537	41.51	14.48_6	0.0578	0.0081	0.0037	0.0111	14.59*	0.421
0.00	101.3	648993	5.537	41.51	14.91_7	.0578	.0083	.0038	.0114	15.03	17.86
75.00	101.3	728794	5.529	43.22	17.41_7	.0850	.0095	.0044	.0132	17.56	14.01
Nitrogen											
9.60	1.01	109567	5.536	41.96	2.545_2	0.0611	0.0016	0.0006	0.0015	2.488	1.2
9.60	101.3	134307	5.536	41.96	3.119_9	.0611	.0019	.0008	.0020	3.065	121.5
75.00	1.01	126009	5.529	43.22	3.011_4	.0850	.0018	.0007	.0018	2.932	0.98
75.00	101.3	143527	5.529	43.22	3.430_0	.0850	.0021	.0009	.0023	3.353	95.4
75.00	253.3	176387	5.529	43.22	4.215_3	.0850	.0025	.0011	.0129	4.143	217.0

*Corrected for temperature jump, $K=14.61\times10^{-2}$ w m^{-1} K^{-1}.

The uncertainty of the results at the 99 percent confidence level is estimated to be ±0.7 percent and is derived as the root of the sum of the squares of the estimates of the 3 σ errors of the following:

Estimate of the error in the value of the

Cell constant	$3\sigma=\pm0.1$ %
Emitter power	$3\sigma=\pm0.1$ %
Extrapolation to ψ_0	$3\sigma=\pm0.45$%
Temperature rise	$3\sigma=\pm0.45$%
"Vacuum conductivity"	$3\sigma=+0.004\times10^{-2}$ w m^{-1} K^{-1}

3. Discussion

According to the kinetic theory of gases, the ratio $f=K/(\eta c_v)$, should be [3]

$$f=2.5f_\lambda^{(3)}/f_\eta^{(3)}$$

for a monatomic gas. The value of $f_\lambda^{(3)}/f_\eta^{(3)}$ depends upon the potential function of the particular atom and is only about 3×10^{-3} greater than unity for helium. For the value of helium reported for 0 °C and 2.39×10^5 Pa, adjusted to zero pressure, and for the heat capacity at constant volume of 3/2 R per mol, the value of f is

$$f=14.60\times10^{-2}\times0.0040026/(1.86885\times10^{-5}\times8.3143\times1.5)=2.5073.$$

The value of the viscosity was derived from publications by Kestin et al. [5, 6, 7], and the value of the gas constant was taken from an evaluation of the fundamental constants [8]. The calculated value of the ratio, where the values of $f_\lambda^{(3)}$ and $f_\eta^{(3)}$ are derived for the same potential parameter given for the viscosity, is 2.5085. Thus the values from experiment and theory are in agreement within 0.05 percent, much less than the experimental uncertainties.

For many gases the increase of the thermal conductivity with pressure is principally a function of density. The increase found for helium at 0 °C is $\partial K/\partial\rho=2.41\times10^{-4}$ in the units of table 3. When the pressure effect is deducted from the thermal conductivity value found for helium at 75.00 °C and 1.01×10^7 Pa pressure, the value of K for the same temperature and zero pressure is 17.22×10^{-2} w m^{-1} K^{-1}. Kestin's experimental value for the viscosity of helium at 75.00 °C is 22.07 kg m^{-1} s^{-1}, so that $f=2.5042$, for the derived value of helium, an agreement with the theoretical value of 2.5085 that must be somewhat fortuitous.

The author suggests that most thermal conductivity values for helium are low because of contamination by degassing of the apparatus. Such an effect would diminish with pressure, and might be confused with "temperature jump" effects. The length of the temperature jump is [9]

$$g=\frac{2-a}{a}\frac{4c}{\gamma+1}\frac{K}{\eta c_v}L$$

where a is the thermal accommodation coefficient, $0.491\leq c\leq0.499$, $\gamma=c_p/c_v$, and L is the mean free path. When a is taken to be 0.37 [10], the value of g is about 8 L. At 10^5 Pa pressure and 0 °C, $L=12\times10^{-6}$ cm, so that the relative effect of the temperature jump on the heat transfer in the M. I. T. cell amounts to 2.8×10^{-3}. Probably the uncertainty of the theory of the temperature jump should be assumed to be 20 or 25 percent. A correction to the conductivity of helium calculated for the effects of temperature jump at 1 atm involves too much uncertainty, hence the choice of 2.39×10^5 Pa, at which pressure the reduction of heat transfer from temperature jump in the cell is calculated to be 1.2 parts per thousand. On the other hand, for both nitrogen and argon the effects of temperature jump at one atmosphere pressure and 0 °C are calculated to be less than 0.5 part per thousand.

A similar calculation of $f=K/(\eta c_v)$ for argon gave the value of 2.506 at 0 and 2.500 at 25 °C, when the values of the viscosities were derived from the work of DiPippo and Kestin [7]. The viscosity values used were 21.10 kg m^{-1} s^{-1} at 0 °C and 22.21 kg m^{-1} s^{-1} at 25 °C. The value of $f_\lambda^{(3)}/f_\eta^{(3)}$ for argon is about 1.001 in this temperature range, so that the theoretical value of f is 2.503. The viscosity results published by Kestin et al. are likely to be so accurate that the discrepancies between experimentally and theoretically derived values of f will come predominantly from errors in the measurement of the thermal conductivities. The agreement of the experimentally derived values of f with the theoretically derived values is within 0.12 percent, distinctly less than the uncertainties to be expected for the most accurate measurements of thermal conductivities.

The determination of the thermal conductivities of gases at high densities is apt to be erroneously high because of heat transfer by convection. It has been expected that the parallel plate cell, with the conductivity gap horizontal and the emitter plate above the receiver, would be free of the effects of convection. The accurate performance of a thermal conductivity cell in this configuration has been attained by Michels and Sengers [11]. Heat transfer by convection was expected for our coaxial cylinder cell. The measurements were made as a function of temperature rise so that the resulting data could be extrapolated to zero temperature rise; the effects of convection, so long as it was entirely laminar, could thereby be eliminated. Heat transfer by laminar convection in a vertical coaxial cylinder cell will not significantly involve the emitter if the conductivity gap is sufficiently extended in each direction by long guards. Such equipment has been used by Ziebland [12], and Johannin, Le Neindre and other workers at the Laboratoire des Hautes Pressions of the CNRS at Bellevue, France [13, 14]. A large fraction of thermal conductivity measurements at high density, however, have been reported for equipment for which neither adequate experimental precautions nor appropriate treatment of data were used.

At low densities, the thermal conductivity of nitrogen has been accurately measured also by Nuttall and Ginnings [15], and Michels and Botzen [16]. Within the stated experimental errors, their values and the low density values reported in this paper are in agreement.

The additional thermal conductivity of nitrogen due to pressure, the "excess thermal conductivity", appears to be a function of density only. The data for figure 1 are given in table 4, which covers measurements from 0 to 700 °C, and pressures up to 1.3×10^8 Pa (1284 atm).

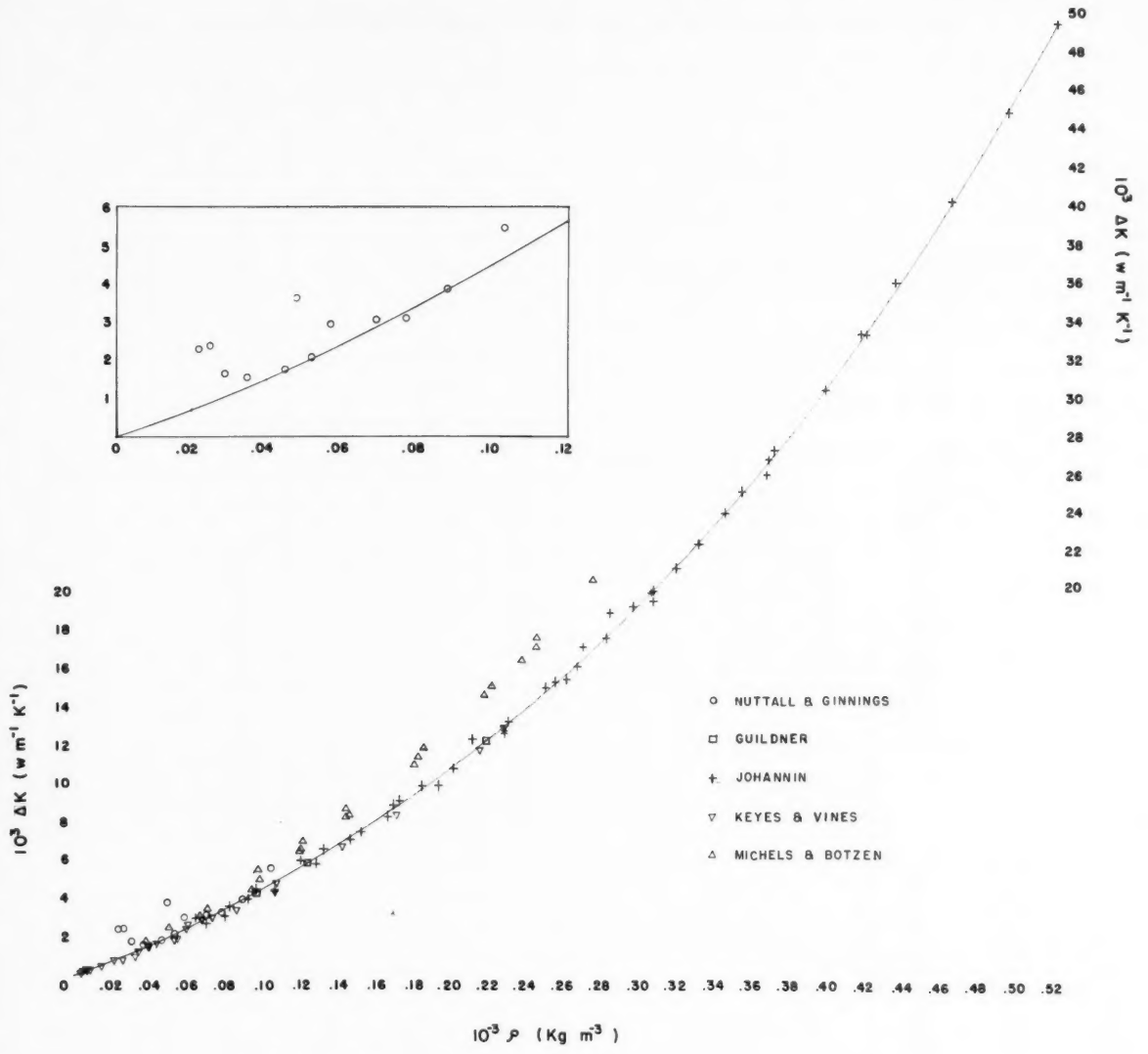

FIGURE 1. *The excess thermal conductivity of nitrogen versus its density.*

The data are obtained from various papers reporting measurements made at temperatures from 0 to 700 °C, and at pressures from 1×10^5 to 1.3×10^8 Pa.

TABLE 4. *The excess thermal conductivity of nitrogen at higher pressures*

Guildner

9.6 °C

10^{-5} P (Pa)	10^{-3} ρ (kg/m^3)	10^3 ΔK (w m^{-1} K^{-1})
101.3	0.122	5.77

75 °C

101.3	0.0954	4.21
253.3	.217	12.11

Michels and Botzen

25 °C			50 °C		
P	ρ	ΔK	P	ρ	ΔK
1	0.00114	0	1	0.00106	0
10.5	.0119	0.5	12.4	.0129	.6
21.8	.0217	0.9	34.2	.0356	1.5
33.0	.0367	1.7	63.4	.0656	3.0
43.3	.0491	2.4	94.3	.0969	4.9
61.6	.0697	3.4	118.0	.120	6.9
85.0	.0960	5.4	142.6	.143	8.6
106.1	.119	6.5	188.0	.184	11.8
128.6	.143	8.2	231.1	.220	15.0
163.2	.179	10.9	262.1	.244	17.5
202.7	.216	14.5			
224.1	.236	16.3			
270.0	.274	20.5			

75 °C

1	0.00098	0
12.6	.0121	.4
37.1	.0356	1.3
74.2	.0705	3.0
99.1	.0934	4.4
127.1	.118	6.4
157.8	.145	8.3
202.5	.181	11.3
244.4	.216	14.5
258.4	.244	17.0

Nuttall and Ginnings

	10^{-5} P = 50.6 Pa		10^{-5} P = 101.3 Pa	
t °C	ρ	ΔK	ρ	ΔK
50	0.052	2.09	0.103	5.44
100	.045	1.76	.088	3.85
150			.077	3.10
200	.035	1.55	.069	3.06
300	.029	1.67	.057	2.97
400	.025	2.39	.048	3.64
500	.022	2.30		

Values of the densities were derived from numerous *PVT* data, and are probably not in error more than ±1 percent. Most of the values of ΔK are those published by Keyes and Vines [17].

P. Johannin

75 °C			125 °C		
P	ρ	ΔK	P	ρ	ΔK
102	0.095	4.4	100	0.081	3.5
181	.171	9.0	196	.151	7.4
390	.305	19.8	390	.266	16.0
588	.397	30.4	588	.353	25.1
782	.464	40.2	782	.419	33.3
977	.520	49.4	1039	.494	44.8
200 °C			300 °C		
101	0.069	2.6	197	0.105	4.3
198	.127	5.7	396	.192	9.8
395	.227	12.6	588	.260	15.3
593	.306	19.4	782	.318	21.1
782	.366	26.0	977	.367	26.8
977	.416	33.3	1301	.434	36.0
400 °C			500 °C		
198	0.091	3.9	196	0.079	3.0
391	.165	8.2	390	.145	7.0
584	.227	12.6	577	.200	10.7
780	.281	17.5	787	.254	15.2
984	.330	22.4	1024	.306	19.9
1172	.370	27.3	1217	.344	24.0
600 °C			700 °C		
197	0.070	3.0	197	0.063	2.9
392	.131	6.5	395	.119	5.9
588	.183	9.8	590	.168	8.8
782	.229	13.1	783	.210	12.2
973	.269	17.0	978	.249	14.9
1111	.295	19.1	1173	.283	18.8

Keyes and Vines [17]

139.70 °C			249.40 °C		
P	ρ	ΔK	P	ρ	ΔK
4.48	0.0036	0.17	3.45	0.0022	0.04
6.89	.0056	0.29	20.68	.0132	0.42
37.57	.0303	1.21	49.49	.0312	0.84
47.57	.0382	1.55	83.42	.0518	1.76
51.36	.0412	1.59	86.18	.0534	1.84
73.77	.0585	2.39	139.9	.0846	3.26
75.15	.0596	2.51	177.5	.105	4.27
139.2	.106	4.73	303.4	.170	8.29
190.3	.141	6.62	434.4	.227	12.81
317.1	.214	11.64			
196.75 °C			300.90 °C		
7.58	0.0055	0.13	12.07	0.007	0.21
34.14	.0245	0.67	35.16	.020	0.71
			68.94	.039	1.55
			131.0	.072	2.89
347.60 °C					
13.45	0.007	0.29			
34.45	.018	0.75			
69.63	.037	1.55			
129.3	.066	2.93			

The values reported for higher densities in [15] and [16] are inconsistent with other data. The satisfactory correlation of the Keyes and Vines data tends to substantiate that the work and treatment of data may have been satisfactory, but adequate information is lacking in the paper itself.

Good measurements of the thermal conductivity of argon were made by Michels et al [18]. The values at 0 and 25 °C for a pressure of 1×10^5 Pa atmosphere are 1.633×10^{-2} w m^{-1} K^{-1} and 1.758×10^{-2} w m^{-1} K^{-1}, differing from the results in this paper by -1.1 percent and -0.4 percent, respectively. The increase of thermal conductivity at 0, 25, 50, and 75 °C for pressure increases up to 2.46×10^8 Pa (2424 atm) can be satisfactorily correlated as a function of density only.

4. Conclusions

When careful work is combined with well-designed equipment, the thermal conductivities of gases can be determined with an uncertainty of less than 1 percent even at high pressures. For the noble gases, the thermal conductivities measured for He and Ar at low density are entirely consistent with the predictions of the kinetic theory, and similar agreement can be expected for Ne, Kr, and Xe. The increase of the thermal conductivity as the gas density increases is found to be a function of density only for nitrogen in the range of 0–700 °C and up to 1.301×10^8 Pa (1284 atm) pressure.

Note added in proof:

A trade name is used in this manuscript. In no case does such identification imply recommendation or endorsement by the National Bureau of Standards.

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On the Differential Cross Section for X-Ray Inelastic Scattering

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A formal formulation of the differential cross section for x-ray inelastic scattering is given for a real solid, in particular, in terms of the polarization propagator and the inverse dielectric function. The differential cross section is related to the causal functions of electron properties rather than those retarded functions.

Key words: Differential cross section; real metals; theory; x-ray inelastic scattering.

A few years ago, the present author formulated the differential cross section for x-ray inelastic scattering in a unified way such that core electrons as well as valence electrons were treated on an equal basis [1].[1] This formulation aided explanation of the then unresolved x-ray Raman scattering problem. In this paper, the differential cross section will be expressed in terms of causal rather than retarded functions in model-independent form. The results are similar in form to the Noziéres-Pines [2] results for an electron gas in the dielectric formulation.

Several results of this paper have been reported previously or used separately in papers published elsewhere [3, 4]. It is, however, desirable to present the entire formulation in a systematic way, although the formulation is a trivial one to those who are familiar with Schwinger's many-body formulation and the spectral function technique.

In previous papers [1, 5] it was shown that the differential cross section for x-ray inelastic scattering is given by the double four-dimensional Fourier transform of the electron charge (or current) correlation:

$$\sigma(k\to k') \equiv C(k,k')(\boldsymbol{\epsilon}\cdot\boldsymbol{\epsilon}')^2 \int\int d^4x\, d^4y\, \langle \Delta\rho(x)\Delta\rho(y)\rangle \exp\,[-i(k-k')(x-y)], \tag{1-a}$$

where k and k' are the four-vectors consisting of the wave vectors and the energies of the incoming and the outgoing photons, respectively, and $\boldsymbol{\epsilon}$ and $\boldsymbol{\epsilon}'$ are their polarization directions. The quantity $C(k,k')$ is defined by

$$C(k,k') = (2\pi)^{-4}(e^2/m)^2(kk')^{-1}. \tag{1-b}$$

The function $\rho(x)$ is the electron charge operator and $\Delta\rho(x)$ is given by

$$\Delta\rho(x) = \rho(x) - \langle\rho(x)\rangle, \tag{2}$$

where $\langle Q\rangle$ indicates the expectation value of an operator Q with respect to the ground (Fermi vacuum) state of the electron system. This ground state[2] is a Heisenberg state of the electron system in the absence of radiation fields [1]. Units are such that $\hbar = c = 1$ and the metric is $kx = \mathbf{k}\cdot\mathbf{r} - |k|t$ if the four vectors are given by $k = (\mathbf{k}, |k|)$ and $x = (\mathbf{r}, t)$.

Since the charge correlation in eq (1) is defined by the Fermi vacuum expectation value of the system of electrons per se, one can proceed via the standard approach for many interacting electron problems to calculate it. In particular, we use Schwinger's action principle [6] by adding an external c-number source function to the Hamiltonian density of the electron system. The Hamiltonian density due to the external source, $U(x)$, is given by

$$\mathscr{H}_S(x) = U(x)\psi^+(x)\psi(x), \tag{3}$$

where $\psi(x)$ is the electron field operator and $\psi^+(x)$ is its adjoint. Then the action principle gives

$$i\frac{\delta\langle Q(1)\rangle}{\delta U(2)} = \langle T[Q(1)\psi^+(2)\psi(2)]\rangle - \langle Q(1)\rangle\ \langle\psi^+(2)\psi(2)\rangle \tag{4}$$

[1] Figures in brackets indicate the literature references at the end of this paper.
[2] At finite temperatures, the ground state average $\langle \ldots \rangle$ must be replaced by an average over a grand canonical ensemble.

where the variable, say 1, is short for $x_1=(\mathbf{r}_1, t_1)$; $Q(x)$ is any operator in the Heisenberg representation; the symbol $T[\ldots]$ implies the time ordering operation for fermions. The electron Green's function is defined by

$$G(12)=(-i)\ \langle T[\psi(1)\psi^+(2)]\rangle\ . \tag{5}$$

From this, the vacuum expectation value of the electron charge operator, $\rho(x)$, is given by

$$\langle \rho(1)\rangle\ =\ \langle \psi^+(1_+)\psi(1)\rangle\ =(-i)G(1,1_+), \tag{6}$$

where 1_+ indicates the four vector $(\mathbf{r}_1, t_1+0)$.

If we substitute (6) into (4), we obtain

$$iS(12)\equiv i\,\frac{\delta\ \langle \rho(1)\rangle}{\delta U(2)}=\frac{\delta G(1,1_+)}{\delta U(2)}=$$

$$\langle T[\Delta\rho(1)\cdot\Delta\rho(2)]\rangle\ . \tag{7}$$

This quantity is a causal Green's function, while the quantity in eq (1) is merely a time correlation. These two are, of course, different functions. However, there is a definite mathematical relation between them in the spectral representation [7, 8], provided that translational time invariance holds. In our electron system, this invariance holds since the total Hamiltonian of the electron system is thought of as being time independent.

At absolute zero,[3] the spectral relationship between the time correlation and the causal function is given by

$$\langle\Delta\rho(1)\Delta\rho(2)\rangle_\omega=-2\mathrm{Im}[(-i)\langle T[\Delta\rho(1)\Delta\rho(2)]\rangle_\omega], \tag{8}$$

where $\langle\ldots\rangle_\omega$ implies the spectral intensity (the Fourier transform using a basis of $\exp[-i\omega(t_1-t_2)]$) of the function $\langle\ldots\rangle$, and the symbol Im denotes "the imaginary part of". Since the differential cross section, eq (1), contains the quantity given by eq (8), we now study the properties of the causal function eq (7).

The electron system which we are dealing with must represent that of a real crystal. In such a system translational invariance may not hold for spatial coordinates. Therefore we deal with quantities, such as eq (7), as they are written, in terms of space-time coordinates; but not in terms of their Fourier transform until we reach the very end. The electron Green's function, G(12), satisfies the electron Green's function equation:

$$G^{-1}(1\bar{1})G(\bar{1}2)=G(1\bar{1})G^{-1}(\bar{1}2)=\delta(12), \tag{9}$$

where the convention for integrations applies to the repeated variables with a bar. The vertex function for electron-electron interaction (not a radiation part) is defined by

$$\Gamma_U(12;3)=\frac{\delta G^{-1}(12)}{\delta U(3)} \tag{10}$$

The quantity G^{-1} can be given in terms of the total average potential, $V(1)$, of the system and the self-energy operator $\Sigma(12)$:

$$G^{-1}(12)=\left[i\frac{\partial}{\partial t_1}+\frac{\nabla^2(1)}{2m}+\sum_n Z_n v_c(1,\mathbf{R}_n)+\mathscr{E}_f\right]\delta(12)$$

$$-V(1)\ \delta(12)-\Sigma(12), \tag{11}$$

and

$$V(1)=U(1)-iv_c(1\bar{1})\,G(\bar{1}\,\bar{1}_+), \tag{12}$$

where $\mathbf{R}_n$ denotes the position of the nucleus n, $Z_n|e|$ is the charge of the nth nucleus, v_c is the instantaneous Coulomb interaction, and $\mathscr{E}_f$ is the Fermi energy. The self energy operator Σ is given by

$$\sum(12)=-i\,v_c(1\bar{1})G(1\bar{2})\,\Gamma_U(\bar{2}2;\bar{1}_+). \tag{13}$$

The time ordered product of $\Delta\rho$ has been connected to the variational derivative of the electron Green's function by eq (7). In terms of the vertex function, eq (10), we can write

$$S(12)=i\,G(1\bar{1})\,\Gamma_U(\bar{1}\,\bar{2};2)\,G(\bar{2}1_+). \tag{14}$$

This expression provides a way of calculating the charge correlation from eq (7). However, there is another way [9] to express it, emphasizing the dynamic properties of interacting electrons. Such dynamic properties of electrons can be characterized by a generalized dielectric or inverse dielectric function of the system, which represents the true response of the system, including the dynamic screening effect of electron interactions. The inverse dielectric function can be defined by

$$\epsilon^{-1}(12)=\frac{\delta V(1)}{\delta U(2)}. \tag{15}$$

Then we obtain

$$S(12)=P(1\bar{1})\,\epsilon^{-1}(\bar{1}2), \tag{16}$$

where P is the irreducible polarization propagator [9, 10]. This propagator is now given in terms of a new dressed vertex function Γ by

$$P(12)=i\,G(1\bar{1})\Gamma(\bar{1}\bar{2};2)G(\bar{2}1_+), \tag{17}$$

where

$$\Gamma(12;3)=\frac{\delta G^{-1}(12)}{\delta V(3)}. \tag{18}$$

[3] At finite temperatures, the right-hand side of eq (8) should be multiplied by the following factor

$$f(\omega,T)=\frac{1}{1+\eta\exp[-\omega/kT]}, \tag{8'}$$

where T is absolute temperature, k is Boltzmann's constant and η is -1 for fermions.

We have thus calculated the causal function $S(12)$ originally defined by eq (7). We have also found that the spectral intensity of the time correlation is related to that of the causal function by relation (8). Since the differential cross section (1–a) is given by the Fourier transform of the electron charge time-correlation, it is now possible to calculate the differential cross section (1–a) from the causal function $S(12)$ through eq (16). We write the double Fourier transform of function $F(12)$ as follows:

$$F(12) = \int \frac{d\omega}{2\pi} \frac{d\mathbf{k}_1}{(2\pi)^3} \frac{d\mathbf{k}_2}{(2\pi)^3} F(\mathbf{k}_1, \mathbf{k}_2; \omega) \exp[i\mathbf{k}_1\mathbf{r}_1 - i\mathbf{k}_2 r_2 - i\omega(t_1 - t_2)]. \tag{19}$$

In terms of these Fourier transforms, eq (8) gives

$$N(\mathbf{k}_1, \mathbf{k}_2; \omega) = -2 \operatorname{Im} S(\mathbf{k}_1, \mathbf{k}_2; \omega), \tag{20}$$

where $N(\mathbf{k}_1, \mathbf{k}_2; \omega)$ is the Fourier transform of the charge correlation $\langle \Delta\rho(x)\Delta\rho(y)\rangle$. It is convenient at this stage to introduce two experimental variables. One is the momentum transfer κ which is given by both the energy (or wave-length λ_{in}) of the incoming x rays and the scattering angle θ. The other is the energy transfer E which is the energy loss of the outgoing x rays. These quantities are defined by

$$\boldsymbol{\kappa} = \mathbf{k} - \mathbf{k}'; \quad |\boldsymbol{\kappa}| \simeq (4\pi/\lambda_{in}) \sin(\theta/2) \tag{21}$$

and

$$E = |\mathbf{k}| - |\mathbf{k}'|. \tag{22}$$

Then the differential cross section (1–a) is rewritten in terms of the double Fourier transform of the charge correlation, $N(\boldsymbol{\kappa}, \boldsymbol{\kappa}, E)$ as

$$\sigma(k \to k') \equiv \sigma(\boldsymbol{\kappa}, E) = C(k, k')(\boldsymbol{\epsilon}\cdot\boldsymbol{\epsilon}')^2 \int dt\, N(\boldsymbol{\kappa}, \boldsymbol{\kappa}; E). \tag{23}$$

It should be noted that the differential cross section defined by (1–a) is the *total* transition probability instead of the customary transition probability per unit time (i.e., rate). As seen from (23), the customary transition rate $\bar{\sigma}(\boldsymbol{\kappa}, E)$ is given by the integrand of eq (23) since the integrand turns out to be time independent:

$$\sigma(\boldsymbol{\kappa}, E) = \int dt\, \bar{\sigma}(\boldsymbol{\kappa}, E). \tag{24}$$

Finally the customary differential cross section is given via eq (20) by

$$\bar{\sigma}(\boldsymbol{\kappa}, E) = (-2)\, C(kk')\, (\boldsymbol{\epsilon}\cdot\boldsymbol{\epsilon}')^2 \operatorname{Im}\left[\int \frac{d^3k}{(2\pi)^3} P(\boldsymbol{\kappa}, \bar{\mathbf{k}}; E)\, \epsilon^{-1}(\bar{\mathbf{k}}, \boldsymbol{\kappa}; E)\right], \tag{25}$$

where the Fourier transform of eq (16) is used to express $S(\boldsymbol{\kappa}, \boldsymbol{\kappa}, E)$. This expression has been used to calculate the inelastic scattering profiles at different scattering angles in both the Hartree-Fock and the random phase approximations [3, 4].

As mentioned previously, the present formulation is model-independent and also holds for real crystals. In such crystals, periodic spatial translational invariance may not hold, thus forbidding the use of a Fourier series-integral expansion. As seen in the expression of the differential cross section, the final result is given by the double Fourier transforms of the physical quantities. Even in the crystal with imperfect spatial translational invariance, one can always expand the nonlocal functions by the double Fourier integrals as we have shown here.

Another advantage of the present result is found in its capability of separating, for instance, the core electron contribution from the valence electron contribution, thus filling in the gap between the modern x-ray inelastic theory and the traditional Waller-Hartree expression [11]. This separation can be done, because the polarization propagator, P, can be expressed as a sum of two terms: $P = P_{core} + P_{valence}$. It is also possible to deal with the interaction of electrons in crystals realistically through a proper decomposition of the P: for instance, $P = P_{diagonal} + P_{nondiagonal}$.

As a final point, note that, substituting expression (12) into (15), we obtain

$$\epsilon^{-1}(12) = \delta(12) + v_c(1\bar{1})\, S(\bar{1}2). \tag{15'}$$

The Coulomb potential, $v_c(12)$, is instantaneous and a function of **1–2**. Therefore, the Fourier transform of v_c can be diagonalized. Utilizing this property, one may express the imaginary part of $S(12)$ by that of $\epsilon^{-1}(12)$, like in an electron gas model.

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Simplification of van der Poel's Formula for the Shear Modulus of a Particulate Composite

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The coefficients in van der Poel's equation for calculating the shear modulus of a particulate composite have been greatly simplified, making the calculation much less unwieldy. Approximate solutions of van der Poel's equation are also derived, and it is shown that one of the low order approximations is Kerner's equation, or Hashin and Shtrikman's equation for the highest lower bound. The Kerner approximation is often too low in value when the volume fraction of filler exceeds 0.2, but it can be used to provide further simplification in van der Poel's equation, or it can be used as a first approximation in a Newton's method of solution.

Key words: Composite materials; elastic constants; filled polymers; mechanical properties; particulate composites; shear modulus; theory of elasticity.

1. Introduction

Van der Poel's method [1][1] for calculating the shear modulus of a particulate composite is an excellent method capable of giving accurate results [1, 2], but because of several disadvantages has not been widely used. In the original presentation the calculation was complicated. A table of values was therefore provided, but this table was limited to materials for which Poisson's ratio of the matrix was 0.5. In addition, there was an error in the derivation [3], and its effect on the results was not known. Recently, however, van der Poel's method has been reexamined [4], the error corrected, and the method extended for use with matrix materials having any value for Poisson's ratio. The effect of the error was shown to be minor, and a new table of values was provided. Continued studies have now resulted in an improved understanding of the theory, and have provided significant simplifications in the calculation. This work is presented here.

2. Review of the Method

A detailed derivation based upon a method developed by Frölich and Sack [5] has been given elsewhere [4]. Consider an idealized composite material consisting of small spheres imbedded in a matrix. The spheres are of approximately the same size, are firmly attached to the matrix, and are uniformly distributed so that the composite material is macroscopically homogeneous and isotropic. To simplify calculations consider a unit length chosen such that on the average there is one sphere of filler in each spherical volume $4\pi/3$ of unit radius. If a is the radius of the filler sphere, then by definition of the unit radius, a^3 is equal to the volume fraction φ of the filler.

Consider a large sphere of homogeneous material. Consider also a second sphere of the same size consisting mostly of the homogeneous material but having the following structure in the central region: A filler sphere of radius a is located at the origin. Surrounding this out to a radius unity is a shell of matrix material, which in turn is imbedded in the homogeneous material. The mechanical properties of this homogeneous material are assumed to be the same as the average macroscopic properties that are sought for the composite material considered here.

If the same boundary stresses are applied to each of the spheres, it is assumed that the displacements in the two spheres will be the same at a distance $r \gg 1$, except for terms of a high order in $1/r$. Thus it is required that

$$\frac{\text{Displacement at } r \gg 1 \text{ in second sphere}}{\text{Displacement at } r \gg 1 \text{ in first sphere}} = 1 + \sum_{n>3} \frac{\text{Const.}}{r^n} \quad (1)$$

Let the first sphere be subjected at the boundary to the deviatoric stress system

$$\sigma_r = 2TP_2(\text{Cos } \theta), \qquad \tau_{r\theta} = TP_2'(\text{Cos } \theta), \qquad \tau_{r\phi} = 0. \quad (2)$$

[1] Figures in brackets indicate literature references at the end of this paper.

where σ_r is the radial tensile stress, and $\tau_{r\theta}$ and $\tau_{r\phi}$ are the tangential shear stresses on the spherical boundary surface at radius r. The corresponding boundary displacements in the r, θ, and ϕ directions are

$$u_r=\frac{Tr}{G}P_2(\text{Cos }\theta),\ u_\theta=\frac{Tr}{2G}P_2'(\text{Cos }\theta),\ u_\phi=0. \quad (3)$$

In the above equations T is a stress magnitude, and G is the shear or rigidity modulus. $P_2(\text{Cos }\theta)$ is the second Legendre Polynomial, and $P_2'(\text{Cos }\theta)$ is its derivative with respect to θ.

The stresses and displacements at any radius r within sphere 1 of the homogeneous material are also given by eqs (2, 3), but the stresses and displacements within sphere 2 having the special structure must be found by solving Lamé's equations. These solutions subject to the requirement of symmetry about the $\theta=0$. axis, and the requirement that the solutions possess the same P_2 symmetry as those of eqs (2, 3), have been derived in the previous paper [4] and are given by

$$u_r=[A_m r+B_m r^{-4}+C_m r^3+D_m r^{-2}]P_2(\text{Cos }\theta) \quad (4)$$

$$u_\theta=\left[\frac{1}{2}A_m r-\frac{1}{3}B_m r^{-4}+\frac{7-4\nu_m}{12\nu_m}C_m r^3+\frac{1-2\nu_m}{5-4\nu_m}D_m r^{-2}\right]P_2'(\text{Cos }\theta) \quad (5)$$

$$\sigma_r=2G_m\left[A_m-4B_m r^{-5}-\frac{1}{2}C_m r^2-\frac{2(5-\nu_m)}{5-4\nu_m}D_m r^{-3}\right]P_2(\text{Cos }\theta) \quad (6)$$

$$\tau_{r\theta}=G_m\left[A_m+\frac{8}{3}B_m r^{-5}+\frac{7+2\nu_m}{6\nu_m}C_m r^2+\frac{2(1+\nu_m)}{5-4\nu_m}D_m r^{-3}\right]P_2'(\text{Cos }\theta) \quad (7)$$

where the quantity ν is Poisson's ratio.

In the above solutions the subscript m refers to the matrix medium of the region $a\leq r\leq 1$ in which these equations hold. Similar equations holding within the filler sphere $r\leq a$ are designated by the subscript f, but in order that these solutions be finite at the origin the coefficients B_f and D_f are set equal to zero. For solutions holding in the region $r\geq 1$ outside the matrix shell no subscripts are used. In these solutions the coefficients C and D do not appear because of the requirement eq (1), and the coefficient A is set equal to T/G for consistency with the applied boundary stresses, eq (2).

At the boundaries $r=a$ and $r=1$. continuity of stress and displacement is required. This results in a system of eight equations in the seven unknowns A_f, C_f, A_m, B_m, C_m, D_m, B, assuming for the moment that the shear modulus G is known. If T is considered as an additional unknown, a system of linear homogeneous equations results. In order that the solution of this system be nontrivial, or that A_f, C_f, A_m, etc. can be expressed in terms of the quantity T, the determinant of the matrix of coefficients must vanish. Setting this determinant equal to zero evaluates G, the shear modulus of the homogeneous material and the quantity sought, in terms of the known quantities G_f, G_m, ν_f, ν_m.

3. Results

The determinantal equation for G can be reduced to the form

$$\alpha X^2+\beta X+\gamma=0. \quad (8)$$

where

$$\alpha=[4P(7-10\nu_m)-Sa^7][Q-(8-10\nu_m)(M-1)a^3]-126P(M-1)a^3(1-a^2)^2 \quad (9)$$

$$\beta=35(1-\nu_m)P[Q-(8-10\nu_m)(M-1)a^3]-15(1-\nu_m)[4P(7-10\nu_m)-Sa^7](M-1)a^3 \quad (10)$$

$$\gamma=-525P(1-\nu_m)^2(M-1)a^3 \quad (11)$$

and the quantities P, Q, and S are defined as

$$P=(7+5\nu_f)M+4(7-10\nu_f) \quad (12)$$

$$Q=(8-10\nu_m)M+7-5\nu_m \quad (13)$$

$$S=35(7+5\nu_f)M(1-\nu_m)-P(7+5\nu_m) \quad (14)$$

M is the ratio G_f/G_m, and the quantity X is equal to $(G/G_m)-1$. Equation (8) has two real roots, one of which is negative and extraneous. The positive root provides the required value for G.

Equations (8) through (11), although more compact than those given previously [4] are still unwieldy, so it becomes worthwhile to search for an approximate solution. Such a solution could be obtained as a series expansion in powers of $a=\varphi^{1/3}$, but in order to obtain sufficient accuracy too many terms would be required. A more compact solution is one of the Padé type:

$$X=\frac{n_0+n_1\lambda+n_2\lambda^2+---}{1+d_1\lambda+\lambda_2\lambda^2+---} \quad (15)$$

where the parameter λ is given by

$$\lambda=\frac{(M-1)a^3}{Q}=\frac{(M-1)\varphi}{Q} \quad (16)$$

To obtain this approximate solution λQ is substituted for $(M-1)a^3$ in eqs (9), (10), (11) for α, β and γ, and these equations are then substituted together with eq (15) into eq (8). The unknown constants n_1, n_2, d_1, d_2, etc. are evaluated by equating to zero the coeffi-

cients of λ in the resulting expression. Several different expansions of the form eq (15) can be obtained, because the pairs of constants n_2, d_1; n_3, d_2; etc. are interrelated. Thus one of the pair members is arbitrary and may be set equal to zero. A suitable approximate expression is

$X_4 =$

$$\frac{15(1-\nu_m)\lambda + 810(1-\nu_m)(1-a^2)^2\lambda^3}{1-(8-10\nu_m)\lambda - 108(1-a^2)^2[8-10\nu_m - 3R/14P]\lambda^3} \tag{17}$$

where R is given by

$$R = 4P(7-10\nu_m) - Sa^7. \tag{18}$$

To a first approximation eq (17) becomes

$$X_1 = \frac{15(1-\nu_m)(M-1)\varphi}{(8-10\nu_m)M + 7 - 5\nu_m}. \tag{19}$$

This approximation has been given previously by Hashin [6], and by Eshelby [7], who found it by different methods. It may be regarded as a generalized form of Smallwood's equation [8].

To a second approximation eq (17) becomes

$$X_2 = \frac{15(1-\nu_m)(M-1)\varphi}{Q-(8-10\nu_m)(M-1)\varphi}. \tag{20}$$

It can be shown by algebraic manipulation that this approximation is the same as Kerner's equation [9], or Hashin and Shtrikman's equation for the highest lower bound [10].

Equation (20) provides a means of further simplifying the exact calculation of X. If the quantities α, β, γ are multiplied by the factor

$$15(1-\nu_m)/[Q-(8-10\nu_m)(M-1)a^3],$$

the following new quantities α', β', γ' are obtained

$$\alpha' = 15(1-\nu_m)R - 126P(1-a^2)^2X_2 \tag{21}$$

$$\beta' = 525P(1-\nu_m)^2 - 15(1-\nu_m)RX_2 \tag{22}$$

$$\gamma' = -525P(1-\nu_m)^2X_2 \tag{23}$$

These new quantities α', β', γ' may be substituted into eq (8) to calculate X.

The approximate solution eq (20) can be used with Newton's method to obtain a better approximation. Let

$$F(X) = \alpha'X^2 + \beta'X + \gamma'$$

$$= \alpha'\left(X + \frac{\beta'}{2\alpha'}\right)^2 - \left(\frac{\beta'^2}{4\alpha'} - \gamma'\right) \tag{24}$$

Then to a first approximation

$$\tilde{F}(X_N) = F(X_2) + (X_N - X_2)F'(X_2) = 0. \tag{25}$$

or

$$X_N = X_2 - \frac{F(X_2)}{F'(X_2)} \tag{26}$$

Evaluating the quantities $F(X_2)$ and $F'(X_2)$ gives

$X_N =$

$$X_2 + \frac{126P(1-a^2)^2X_2^3}{525P(1-\nu_m)^2 + 15(1-\nu_m)RX_2 - 252P(1-a^2)^2X_2^2} \tag{27}$$

The function $F(X)$ is a parabola symmetric about the axis $X = -\beta'/2\alpha'$. At the point where $F(X)$ intersects this axis $F(X)$ is negative. As X increases positively $F(X)$ becomes less negative and is zero where it intersects the X axis. The value of $F(X_2)$ is

$$F(X_2) = -126P(1-a^2)^2X_2^3 \tag{28}$$

and is negative, so that eq (20) provides a value of G less than the true value. On the other hand the value of $F(X_N)$ is

$$F(X_N) = \alpha'(X_N - X_2)^2 \tag{29}$$

and is positive. If X_2 is a sufficiently good approximation, X_N will be an improved approximation, slightly exceeding the true value.

4. Discussion

The exact solution of eq (8) and the approximate solutions eqs (17) and (27) have been studied for volume fractions of filler φ between 0. and 1.0, using the following values for the parameters ν_f, ν_m, and M:

$\nu_f = 0.1$; $\nu_m = 0.4$; $M = 30, 100$
$\nu_f = 0.1$; $\nu_m = 0.5$; $M = 1000$
$\nu_f = 0.25$; $\nu_m = 0.3$; $M = 10$
$\nu_f = 0.25$; $\nu_m = 0.4$; $M = 30, 100$
$\nu_f = 0.25$; $\nu_m = 0.5$; $M = 100, 10^3, 10^4, 7 \times 10^4, \infty$
$\nu_f = 0.35$; $\nu_m = 0.4$; $M = 30, 100$
$\nu_f = 0.35$; $\nu_m = 0.5$; $M = 1000$.

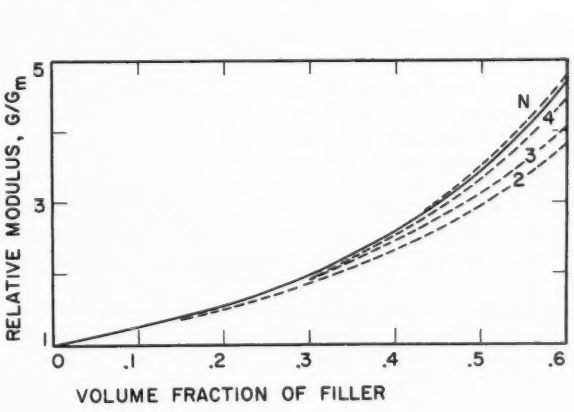

FIGURE 1. *Plot of relative shear modulus* G/G_m *versus volume fraction of filler for the case* $G_f/G_m = 30$, $\nu_f = 0.25$, $\nu_m = 0.40$.

Solid curve, exact solution of eq (8); Dash curve 2, X_2 approximation (Kerner's equation), eq (20); Dash curve 3, X_3 approximation, eq (17); Dash curve 4, X_4 approximation, eq (17); Dash curve N, Newton's method approximation X_N, eq (27).

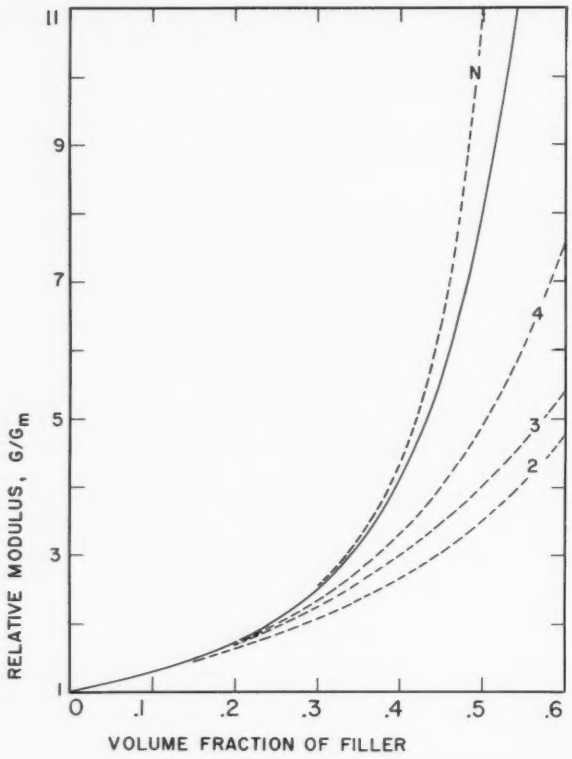

FIGURE 2. *Plot of relative shear modulus* G/G_m *versus volume fraction of filler for the case* $G_f/G_m = 70{,}000$, $\nu_f = 0.25$, $\nu_m = 0.50$.

Solid curve, exact solution of eq (8); Dash curve 2, X_2 approximation (Kerner's equation), eq (20); Dash curve 3, X_3 approximation, eq (17); Dash curve 4, X_4 approximation, eq (17); Dash curve N, Newton's method approximation X_N, eq (27).

Plots selected from these calculations are given for two representative composite materials in figures 1 and 2. In figure 1 the dependence of relative shear modulus G/G_m on the volume fraction of filler φ is shown, as calculated from eqs (8), (17) and (27). The parameter values used were $\nu_f = 0.25$, $\nu_m = 0.4$ and $M = 30$, and are representative of a composite consisting of small glass spheres imbedded in a rigid epoxy matrix. For this example it is seen that the plots for the X_4 and X_N approximations lie reasonably close to either side of the plot for the exact value, but that the plotted values for the X_2 approximation are too low when the volume fraction φ exceeds 0.4.

Figure 2 is a similar plot of values calculated using the parameter values $\nu_f = 0.25$, $\nu_m = 0.50$ and $M = 70{,}000$. These values are representative of a composite consisting of small glass spheres imbedded in a matrix of lightly vulcanized rubber. In this example the X_N approximation calculated from eq (27) gives values close to the exact values calculated from eq (8), when φ is less than 0.4. The approximate values X_2, X_3, X_4 are good only for values of φ up to 0.2.

Equation (16) for the parameter λ may be expressed in the following form

$$\lambda = \frac{\varphi}{8 - 10\nu_m + \dfrac{15(1-\nu_m)}{(M-1)}} \tag{30}$$

When $\nu_m = 0.4$, $M = 30$, $\varphi = 0.4$, the value of λ is $\lambda = 0.09$, and when $\nu_m = 0.5$, $M = 70{,}000$, $\varphi = 0.4$, the value of λ is $\lambda = 0.13$. Thus for values of φ greater than 0.4 the terms in eq (17) representing the successive approximations X_2, X_3, X_4 are relatively large, indicating that this series solution does not converge very rapidly, as evidenced in figures 1 and 2. The approximations provided by eq (17) are probably reliable only for values of φ up to 0.2. In this connection it is appropriate to recall that the approximation X_2 is equivalent to the widely used equation of Kerner [9], or Hashin and Shtrikman's equation for the highest lower bound [10].

It has been pointed out previously that values of G/G_m calculated from van der Poel's equation are insensitive to values of ν_f. The extent of this insensitivity can be seen from eq (17). The values of R and P are moderately dependent on the values of ν_f, and these quantities first appear in the coefficient of λ^3 in the denominator of eq (17). In other words the approximation X_4 is the first one to be affected by the value of ν_f.

Although in the examples of figures 1 and 2 the approximation of eq (27) gives reasonably accurate values, there are situations when eq (27) fails because the approximation X_2 is not good enough. This occurs when for a sufficiently high value of φ the coefficient β', eq (22), changes from a positive to a negative value. The axis of the parabola $F(X) = 0$. then intersects the X axis at the positive point $X = (-\beta')/2\alpha'$. This point will usually be near X_2, and as φ increases will exceed it. In either event the slope $F'(X_2)$ will be too low or even negative, and the calculated value of X_N will be grossly inaccurate.

In the studies using the parameter values listed above, it was found that α' was always positive and γ' was always negative, but when φ exceeded 0.5, β' changed sign and became negative. For values of φ exceeding 0.5 the values of X_N were reasonably accurate when M was less than 100, but when M exceeded 100 the values of X_N were grossly inaccurate or negative.

It is fortunate that eq (27) gives a good approximation for values of φ up to 0.4 or 0.5. At values of φ greater than 0.5 the assumptions upon which the theory is based are no longer valid. For instance, the packing fraction of spheres of equal size arranged on a cubic lattice is 0.52, and the packing fraction of equal size spheres in hexagonal close packed arrangement is 0.74. As a practical matter it is difficult to prepare a particulate composite material with a volume fraction of filler φ exceeding 0.5 without introducing excessive void content. However Schwarzl [2] and van der Poel [1] report that the theory agrees well with experimental data for values of φ up to 0.5. It seems then that the calculations of the theory have an empirical validity beyond the theoretical expectations.

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The Enthalpies of Combustion and Formation of Nicotinic Acid and Creatinine

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The enthalpies of combustion of nicotinic acid and creatinine have been determined in an adiabatic rotating-bomb calorimeter. The enthalpies of formation have been obtained by combination of the experimental data with the accepted values for the enthalpies of formation of carbon dioxide and water. The results of other investigations on creatinine are discussed briefly. The resulting values and their estimated uncertainties are as follows:

	Nicotinic acid	*Creatinine*
$\Delta Hc°(25\ °C)$	-2730.67 ± 0.57 kJ/mol	-2334.53 ± 0.86 kJ/mol
$\Delta Hf°(25\ °C)$	-344.97 ± 0.62 kJ/mol	-239.93 ± 0.88 kJ/mol

Key words: Calorimetry; combustion; creatinine; enthalpy; formation; heat; nicotinic acid.

1. Introduction

This investigation is part of a program to obtain reliable thermodynamic data for important biochemical substances. Nicotinic acid and creatinine are compounds occurring in living processes and have biological as well as biochemical importance. Since nicotinic acid is used as a standard in clinical analyses there is need for reliable thermodynamic data which so far has been non-existent. There is also need for a standard reference material for use in the evaluation of calorimetric and analytical procedures involving nitrogen-containing compounds.

2. Materials

2.1. Benzoic Acid

The benzoic acid used for the calibration experiments and also as an auxiliary material was SRM calorimetric standard 39i obtained from the NBS Office of Standard Reference Materials. The purity of this material was given as 99.997 mole percent and the calorific value was certified to be 26434 J/g under certificate conditions. Conversion to thermodynamic standard state conditions gave $\Delta U_c°(28\ °C)$ as -26410.36 J/g and $\Delta U_c°(26\ °C)$ as -26412.35 J/g.

2.2. Creatinine

The sample of creatinine was obtained from the Office of Standard Reference Materials as SRM 914; it was certified as a chemical of known purity for use in the calibration and standardization of procedures used in clinical analysis. The purity was certified to be 99.8 ± 0.1 percent. The impurities were given as: 0.03 percent volatile matter, 0.07 percent chloride, 0.003 percent ash, and 0.001 percent insoluble matter.

2.3. Nicotinic Acid

The nicotinic acid was obtained from the Office of Standard Reference Materials as SRM 148, a microanalytical standard for use in checking determinations of carbon, hydrogen, and nitrogen. Although the absolute purity has not been established, the titrimetric assay indicates a purity of 99.99 ± 0.08 percent.

All samples were used as received with no attempts at further purification.

2.4. Oxygen

High-purity oxygen was used for both the benzoic acid calibration experiments and the nicotinic acid and creatinine combustion experiments. An analysis furnished with the cylinder showed the following impurities in ppm: Kr, 12.0; Xe, 0.7; N_2O, 0.8; N_2, 3.0; and H_2O, 2.0. The presence of these impurities would have no significant effect on the values obtained for the combustion process.

3. Units and Conversion Factors

The 1969 Table of International Atomic Weights [1][1] was used throughout this paper. The auxiliary data

[1] Figures in brackets indicate the literature references at the end of the paper.

were taken from Selected Values of Chemical Thermodynamic Properties [2]. For conversion to joules from the conventional thermochemical calorie, one calorie was taken as equivalent to 4.1840 joules. All weighings were reduced to weights in vacuum by means of buoyancy corrections derived from air-density determinations.

4. Apparatus and Procedure

The adiabatic rotating-bomb calorimeter, the platinum lined bomb, the adiabatic temperature-control system, the ignition system and the temperature-measurement system have been described [3]. The volume of the empty bomb was 98 cm^3.

The sample was pressed into a pellet and weighed into a platinum crucible using a micro-balance. The crucible, with the sample, was transferred to the crucible support of the bomb which was adjusted so that the sample was in contact with a 2 cm length of 0.075 mm diam platinum wire connected between the bomb electrodes. A small quantity of water (0.30 cm^3 for the benzoic acid calibration experiments and 3.00 cm^3 for the nicotinic acid and creatinine experiments) was added to the bomb which was then sealed, flushed with one liter of oxygen and filled with 31.62 atm of oxygen (1 atm = 101325 N/m^2).

The bomb was placed in the calorimeter, the filling temperature was determined, the calorimeter jacket was evacuated and the adiabatic temperature controls placed in operation. The bomb was then heated electrically to 24.98 °C and the system left overnight for complete thermal equilibrium.

On the following morning temperatures were observed at intervals of a few minutes during a 30-minute initial rating period. The sample was then ignited by discharging a capacitor through the platinum fuse. Two minutes later the bomb was rotated to obtain a homogeneous solution; the rotation was not required for the benzoic acid calibration experiments because of the relatively small amount of nitric acid produced in the combustion. After about 15 minutes, thermal equilibrium was approached and calorimeter temperatures were determined at intervals of a few minutes during a final rating period. Because of the heating effort of the electric current through the platinum resistance therometer there was a constant increase of approximately 0.001 K per hour during the rating periods. The initial and final calorimeter temperatures were obtained by extrapolation of the time-temperature curves for the rating periods to the actual time of ignition.

It was not possible to ignite the creatinine with the platinum fuse; it was necessary to place a very small pellet of benzoic acid on top of the sample with the fuse in contact with the benzoic acid pellet. The fuse then ignited the pellet which in turn ignited the sample. This was not necessary with the nicotinic acid experiments.

The bomb was removed from the calorimeter, and the gaseous contents passed successively through a drying tube and a weighed CO_2-absorption tube. The bomb solution was removed, boiled to expel carbon dioxide, cooled and titrated with standard alkali, using a pH-meter, to determine the quantity of nitric acid produced in the combustion. No trace of nitrous acid was detected.

5. Results and Calculations

The results of the benzoic acid calibration experiments are given in tables 1 and 2 respectively. The calculations were performed by means of a computer program;[2] the values in the tables were taken and rounded from the print-out. The various items in the tables are described as:

EEE-std, the effective energy equivalent of the standard empty calorimeter including the bomb and all internal platinum parts except the crucible at the standard mean temperature of the experiment.

Cv-cont.(i), the heat capacity of all material added to the standard calorimeter, including crucible, sample, oxygen and water.

Corr to *tm*, a correction of 1.8 J/K to the heat capacity of the standard calorimeter for deviation of the actual mean temperature from the standard mean temperature.

Corr-parts, the calculated change in the heat capacity of the calorimeter due to alterations during the series.

[2] A computer program originally prepared by C. H. Shomate of the Naval Ordinance Test Station, China Lake, California, and later modified by G. T. Armstrong and E. J. Prosen, based upon the procedure of Hubbard, Scott, and Waddington [4].

TABLE 1. *Results of the benzoic acid calibration experiments for a temperature rise of 1 °C.*

Expt. No.	505	509	510	511	512	513
EEE-std, J/K	2518.26	2518.24	2517.80	2517.96	2518.19	2517.89
Cv-cont(i), J/K	4.54	4.54	4.54	4.55	4.55	4.52
corr to *std tm*, J/K	.09	.08	.10	.07	.01	.06
corr-parts, J/K	.00	.00	.00	.00	.00	.00
EEE-actual, J/K	2522.89	2522.86	2522.45	2522.57	2522.75	2522.47
Temp rise, K	1.083260	1.064585	1.072635	1.074361	1.014279	1.050943
Q-total, J	−2732.94	−2685.79	−2705.66	−2710.16	−2558.77	−2650.97
q-ign, J	1.08	1.24	1.04	1.08	1.16	1.19
q-decomp HNO_3, J	.09	.08	.08	.08	.12	.12
q-WC, J	2.01	1.97	1.99	2.00	1.89	1.94
q-corr to *std* t_f, J	−.01	−.01	−.01	−.01	.00	−.01
Q-std react, J	−2729.77	−2682.51	−2702.56	−2707.00	−2555.61	−2647.73
m_s	.103352	.101563	.102322	.102490	.096758	.100246
ΔU_c°C (26 °C), J/g	−26412.35	−26412.35	−26412.35	−26412.35	−26412.35	−26412.35
Mean, *EEE-std*, J/K	2518.06					
sdm, J/K	0.08					

TABLE 2. *Results of the benzoic acid calibration experiments for a temperature rise of 3 °C*

Expt. No.	346	347	348	349	350	351	356	357
EEE-std, J/K	2519.04	2519.36	2518.64	2519.21	2518.53	2518.99	2518.62	2518.60
Cv-cont (i), J/K	4.79	4.72	4.74	4.75	4.76	4.75	4.75	4.75
corr to *std tm*, J/K	.41	.06	.13	.11	.16	.12	.13	.12
corr-parts, J/K	.02	.00	.00	.00	.00	.00	.00	.00
EEE-actual, J/K	2524.22	2524.15	2523.52	2524.08	2523.45	2523.86	2523.50	2523.47
Temp rise, K	3.482776	3.054576	3.135678	3.143009	3.166751	3.127852	3.142433	3.131127
Q-total, J	−8791.30	−7710.20	−7912.94	−7933.20	−7991.15	−7894.26	−7929.92	−7901.31
q-ign, J	.93	.86	.83	1.00	.90	.95	1.02	.85
q-decomp HNO_3, J	.14	.35	.51	.32	1.06	.63	.03	.03
q-WC, J	7.24	6.20	6.40	6.44	6.50	6.40	6.43	6.41
q-aux, J	.00	.00	.00	.00	.00	.00	.00	.00
q-corr to *std* t_f, J	−.18	−.02	−.05	−.05	−.06	−.04	−.05	−.05
Q-react, J	−8783.17	−7702.81	−7905.25	−7925.49	−7982.75	−7886.32	−7922.49	−7894.07
m_s, g	.332565	.291659	.299324	.300090	.302258	.298607	.299977	.298900
$\Delta Uc°$ (28 °C), J/g	−26410.36	−26410.36	−26410.36	−26410.36	−26410.36	−26410.36	−26410.36	−26410.36
Mean, *EEE-std*, J/K	2518.88							
sdm, J/K	0.112							

EEE-actual, the effective energy equivalent of the actual, fully loaded, calorimeter at the actual mean temperature of the experiment.

Temp. rise, the difference in K between the initial and final temperatures of the calorimeter obtained by extrapolation of the time-temperature curves to the time of ignition.

Q-total, the total energy absorbed by the calorimeter, obtained as the product of *EEE-actual* in J/K and the temperature rise in K.

q-ign, the quantity of electrical energy introduced into the calorimeter to ignite the sample.

q-decomp HNO_3, the theoretical quantity of energy required to decompose any nitric acid, formed in the combustion, into liquid water and gaseous nitrogen.

q-WC, the Washburn correction [4, 5] applied to convert the contents of the bomb in the initial and final states to their respective thermodynamic standard states.

q-aux, the standard heat of combustion of any auxiliary material, added to insure ignition or to enhance combustion, at the standard final temperature.

q-corr to *std* t_f, a correction to convert the energy evolved by the standard reaction at the actual final temperature to the selected standard final temperature.

Q-std reaction, the energy evolved by the standard reaction at the selected final temperature, obtained as the algebraic sum of *Q-total*, *q-ign*, *q-decomp* HNO_3, *q-WC*, *q-aux*, and *q-corr* to *std* t_f.

m_s, the weight of sample in vacuum.

$\Delta Uc°$, the standard energy of combustion at constant volume at the selected final temperature, obtained as *Q-std* react./m_s.

In the benzoic acid calibration experiments the values for *EEE-std* were calculated by iteration from $\Delta Uc°$. Two series of calibration experiments were used for temperature rises of one and three degrees respectively.

The results of the experiments on nicotinic acid and on creatinine are given in tables 3 and 4, respectively.

The following values[3] were used in the calculations:

	Density, $g \cdot cm^{-3}$	*Cp*, $J \cdot g^{-1} \cdot K^{-1}$	$\left(\frac{\partial U}{\partial P}\right)_t$, $J \cdot g^{-1} \cdot atm^{-1}$
Benzoic acid ...	1.320	1.21	−0.013
Nicotinic acid...	1.47	1.19	− .007
Creatinine.....	1.31	1.23	− .005

The values obtained for nicotinic acid correspond to the process:

$$C_6H_5O_2N(c) + 6.25\ O_2(g) = 6\ CO_2(g) + 0.5\ N_2(g) + 2.5\ H_2O(liq)$$

$\Delta Uc°$ (28 °C) = −22183.27 ± 4.66 J/g
$\Delta Uc°$ (28 °C) = −2731.02 ± 0.57 kJ/mol
$\Delta Hc°$ (28 °C) = −2730.39 ± 0.57 kJ/mol
$\Delta Hc°$ (25 °C) = −2730.67 ± 0.57 kJ/mol
$\Delta Hf°$ (25 °C) = −344.97 ± 0.62 kJ/mol

[3] The densities of nicotinic acid and creatinine were determined by a flotation procedure; the heat capacities and compressibility coefficient of nicotinic acid and creatinine were estimated.

TABLE 3. *Results of the calorimetric combustion experiments on nicotinic acid*

Expt. No.	352	353	354	355	358	359
EEE-std, J/K	2518.88	2518.88	2518.88	2518.88	2518.88	2518.88
Cv-cont(i), J/K	15.94	16.03	16.01	16.02	16.02	4.82
corr to *tm*, J/K	−.49	.10	−.05	.05	.05	−.36
corr parts, J/K	.00	.00	.00	.00	.00	.00
EEE-actual, J/K	2534.33	2535.01	2534.84	2534.94	2534.95	2523.34
Temp rise, K	2.467210	3.128016	2.950755	3.058636	3.076341	2.635465
Q-total, J	−6252.72	−7929.54	−7479.69	−7753.46	−7798.36	−6650.17
q-ign, J	.97	.83	.95	.71	.99	.81
q-decomp HNO_3, J	15.54	19.58	18.13	19.68	19.40	16.52
q-WC, J	9.24	11.89	11.18	11.59	11.67	5.90
q-aux, J	.00	.00	.00	.00	.00	.00
q-corr to *std* t_f, J	0.11	−.03	.01	−.02	−.02	.08
Q-std react, J	−6226.86	−7897.27	−7449.42	−7721.50	−7766.32	−6626.85
m_s	.280691	.356061	.335815	.348040	.350096	.298723
$\Delta Uc°$ (28 °C), J/g	−22184.02	−22179.53	−22183.08	−22185.66	−22183.39	−22183.93
Mean $\Delta Uc°$ (28 °C), J/g	−22183.27					
sdm, J/g	±0.83					

TABLE 4. *Results of the calorimetric combustion experiments on creatinine.*

Expt. No.	500	501	502	503	504	506
EEE-std, J/K	2518.06	2518.06	2518.06	2518.06	2518.06	
Cv-cont(i), J/K	15.73	15.73	15.73	15.73	15.74	15.76
corr to *tm*, J/K	.10	.09	.13	.09	.24	.07
corr parts, J/K	−.01	−.01	−.01	−.01	−.01	−.01
EEE-actual, J/K	2533.89	2533.87	2533.92	2533.87	2534.06	2533.89
Temp rise, K	1.112177	1.097550	1.136384	1.097280	1.264700	1.077063
Q-total, J	−2818.14	−2781.05	−2789.50	−2780.37	−3204.80	−2729.16
q-ign, J	1.22	.89	1.01	1.16	1.01	1.08
q-decomp HNO_3, J	11.78	11.85	12.27	11.60	13.92	10.13
q-WC, J	3.29	3.25	3.38	3.27	3.77	3.21
q-aux, J	240.91	253.65	339.90	370.11	439.81	200.86
q-corr to t_f, J	−.02	−.02	−.02	−.02	−.05	−.01
Q-std react, J	−2560.96	−2511.43	−2522.98	−2394.25	−2746.34	−2513.89
m_s, g	.124008	.121736	.122270	.115978	.133045	.121746
$\Delta U_c°$ (26 °C), J/g	−20651.53	−20630.07	−20634.56	−20644.07	−20642.14	−20648.70
Mean, $\Delta Uc°$ (26 °C), J/g	−20641.84					
sdm, J/g	±3.35					

The values obtained for creatinine correspond to the process:

$$C_4H_7ON_3(c) + 5.25\,O_2(g) = 4\,CO_2(g) + 1.5\,N_2(g) + 3.5\,H_2O(liq)$$

$$\Delta Uc°(26\ °C) = -20641.84 \pm 7.64\ J/g$$
$$\Delta Uc°(26\ °C) = -2334.99 \pm .86\ kJ/mol$$
$$\Delta Hc°(26\ °C) = -2334.37 \pm .86\ kJ/mol$$
$$\Delta Hc°(25\ °C) = -2334.53 \pm .86\ kJ/mol$$
$$\Delta Hf°(25\ °C) = -239.93 \pm .88\ kJ/mol$$

The uncertainties assigned to $\Delta Uc°$ and $\Delta Hc°$ were obtained by combining 2 sdm for the calibration experiments with 2 sdm for the combustion experiments, 0.01 percent for the uncertainty in the certified value for benzoic acid, 0.01 percent for systematic errors and 0.01 percent for the possible effects of impurities in the sample. The uncertainty assigned to ΔHf was obtained by combination of the uncertainty in ΔHc with 0.01 percent in the values taken for the heats of formation of carbon dioxide and water.

The results of the carbon dioxide analyses are given in table 5; the values given were obtained by

$$\frac{CO_2(\text{actual}) - CO_2(\text{theor. for auxiliary})}{CO_2\ (\text{theor. for sample})}$$

TABLE 5. *Results of the CO_2 analyses*

Expt. No.	Nicotinic acid	Expt. No.	Creatinine
352	0.9989	500	0.9950
353	.9988	501	.9954
354	.9984	502	.9978
355	.9981	503	.9980
358	.9993	504	.9983
359	.9995	506	.9972
avg	.9988	avg	.9970

The preliminary work on creatinine showed that when larger samples were used (sufficient to obtain a 3-degree temperature rise) there was evidence of incomplete combustion. Reduction of the amount of sample significantly improved the stoichiometry of the combustion process; the relative amount of benzoic acid used (an auxiliary for ignition) had little or no effect on the stoichiometry.

6. Comparison With Existing Data

Two prior determinations of the enthalpy of combustion of creatinine have been reported. Emery and Benedict [6] obtained the enthalpy of combustion based upon the quantity of carbon dioxide produced in the reaction. Their data was recalculated on the basis of sample weight by Huffman, Ellis, and Fox [7], who also made an independent determination of the enthalpy of combustion. We have corrected these values for changes in atomic weights and have obtained the following values:

$\Delta Hc°$ kJ/mol	
−2328.8 ±5.4	Emery and Benedict [5]
−2335.97 ± 0.67	Huffman, Ellis, and Fox [6]
−2334.53 ± 0.88	This investigation

Huffman, Ellis, and Fox used a paper and platinum wire technique to ignite the sample. They found the samples to be somewhat hygroscopic which may have been due to an electrostatic charge on the pellet.

No previous determinations have been reported on the enthalpy of combustion of nicotinic acid.

7. References

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Simultaneous Measurements of Specific Heat, Electrical Resistivity, and Hemispherical Total Emittance by a Pulse Heating Technique: Hafnium–3 (Wt. %) Zirconium, 1500 to 2400 K*

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(December 20, 1974)

Simultaneous measurements of specific heat, electrical resistivity and hemispherical total emittance of hafnium containing 3.12 weight percent zirconium in the temperature range 1500 to 2400 K by a subsecond duration, pulse heating technique are described. The measurements indicate decreases in specific heat (by about 13%) and in electrical resistivity (by about 8%) as the result of the $\alpha \rightarrow \beta$ transformation. Estimated inaccuracies of the measured properties are: 3 percent for specific heat, 1 percent for electrical resistivity and 5 percent for hemispherical total emittance.

Key words: Electrical resistivity; emittance; hafnium; high-speed measurements; high temperatures; specific heat; thermodynamics.

1. Introduction

In this paper, application of a pulse heating technique to the simultaneous measurements of specific heat, electrical resistivity and hemispherical total emittance of hafnium containing 3.12 weight percent zirconium in the temperature range 1500 to 2400 K is described. For simplicity, in the paper this substance will be referred to as hafnium–3 (wt. %) zirconium. The measurements are of particular interest in view of the fact that hafnium undergoes a solid-solid phase transformation (from hexagonal close-packed to body-centered cubic) in this range.

The method is based on rapid resistive self-heating of the specimen from room temperature to high temperatures (above 1500 K) in less than one second by the passage of an electrical current pulse through it; and on measuring, with millisecond resolution, such experimental quantities as current through the specimen, potential drop across the specimen, and specimen temperature. Details regarding the construction and operation of the measurement system, the methods of measuring experimental quantities, and other pertinent information, such as the formulation of relations for properties, error analysis, etc., are given in earlier publications [1, 2].[1]

In the following sections of this paper a tabular format is adopted in presenting information on the specimen, measurements, system characteristics, results and errors.

2. Measurements

The details regarding the hafnium–3 (wt. %) zirconium specimens used in the present measurements are given in table 1. A summary of the measurement technique and the operational characteristics of the system is given in table 2. The polynomial functions (obtained by the least squares method) that represent the experimental results of specific heat and electrical resistivity are given in table 3. The values of properties at 100 degree temperature intervals computed using the functions are presented in table 4. The experimental results are presented in the appendix. Each number tabulated in the appendix represents results from over 50 original data points. The results of hemispherical total emittance are given in table 7. An estimate of errors in the measured and computed quantities is given in table 5. All values reported in this paper are based on the International Practical Temperature Scale of 1968 [3]. In all computations, the geometrical quantities are based on their room temperature (298 K) dimensions.

*This work was supported in part by the U.S. Air Force Office of Scientific Research.
[1] Figures in brackets indicate the literature references at the end of this paper.

TABLE 1. *Specimen information*

No.	Item	Unit	Explanation
1....	Substance.....	.....	Hafnium–3.12 (wt. %) zirconium.[a]
2....	Source [b]	.....	Materials Research Corporation.
3....	Purity	.....	99.97%.
4....	Impurities	.....	Listed in table 1a.
5....	Geometry	.....	Tube made from rod by electro-erosion.
6....	Dimensions (nominal):		
	total length.....	mm	89.1
	effective [c] length...	mm	38.7
	outside diameter...	mm	6.3
	wall thickness	mm	0.5
	blackbody hole	mm	0.5 × 1 (rectangular)
7....	Weight:		
	total weight.....	g	10.296
	effective [c] weight...	g	4.450
8....	Characteristics:		
	density.....	$g \cdot cm^{-3}$	12.9
	resistivity at 293 K	$10^{-8} \Omega \cdot m$	33.1
9....	Special treatment.....	.....	Heat treated by pulse heating before the experiments—10 pulses to 1700 K.

[a] The analysis to determine the zirconium content was performed by the Spectrochemical Analysis Section at NBS.

[b] The supplier is identified in this paper in order to adequately characterize the specimen—Such an identification does not imply recommendation or endorsement by the National Bureau of Standards.

[c] Effective refers to the portion of the specimen between the voltage probes.

TABLE 1a. *Impurities in the specimen* [a]

(According to the manufacturer's analysis)

Element.....	C	O	N	Al	Ca	Cu	Fe
ppm.....	15	10	10	20	10	10	< 50
Element.....	Mn	Mo	Nb	Si	Ta	Ti	W
ppm.....	20	10	30	20	30	10	10

[a] The total amount of all other detected elements is less than 70 ppm, each element being below 10 ppm limit.

TABLE 2. *Measurement technique and system characteristics*

No.	Item	Unit	Explanation and data
1.....	General technique.....		Pulse heating (subsecond).
2.....	Voltage measurement.....		Across tungsten knife-edge probes.
3.....	Current measurement.....		Across standard resistor (0.001 Ω) in series with the specimen.
4.....	Temperature measurement.....		High-speed photoelectric pyrometer [4].
5.....	Specimen environment.....		Vacuum ~ 1.3×10^{-3} N·m^{-2}(~10^{-5} torr).
6.....	Power source.....		Battery bank (14 series-connected 2V batteries, capacity 1100 A·h each).
7.....	Recording.....		Digital data acquisition system.
8.....	Signal resolution.....		~0.01% (at full scale).
9.....	Time resolution.....	ms	0.4
10.....	Data processing.....		Time-sharing computer.
11.....	Number of specimens.....		2
12.....	Number of experiments.....		11
13.....	Temperature range.....	K	1500–2400
14.....	Experiment duration.....	ms	500–660
15.....	Current pulse length.....	ms	300–460
16.....	Imparted power.....	W	3400–7900
17.....	Current.....	A	700–1000
18.....	Rate of current change.....	A·ms^{-1}	0.1–0.2
19.....	Heating rate.....	K·ms^{-1}	3.7–8.1
20.....	Cooling rate.....	K·ms^{-1}	0.08–0.55
21.....	Radiative heat loss (% of input power).....		2% at 1500 K 8% at 2400 K

TABLE 3. *Functional representation of the results on hafnium–3 (wt. %) zirconium*

Phase	Specific heat (J·g^{-1}·K^{-1})	Electrical resistivity (10^{-8}Ω·m)
α	$1500 < T < 1850$ K $c_p = A + BT$ $A = 1.431 \times 10^{-1}$ $B = 3.830 \times 10^{-5}$ $\sigma^a = 0.3\%$	$1500 < T < 2000$ K $\rho = A + BT + CT^2$ $A = 46.936$ $B = 1.1967 \times 10^{-1}$ $C = -3.0002 \times 10^{-5}$ $\sigma^a = 0.2\%$
β	$2150 < T < 2400$ K $c_p = A + BT + CT^2$ $A = 0.4544$ $B = -2.771 \times 10^{-4}$ $C = 7.286 \times 10^{-8}$ $\sigma^a = 0.5\%$	$2050 < T < 2400$ K $\rho = A + BT$ $A = 130.47$ $B = 1.1276 \times 10^{-2}$ $\sigma^a = 0.2\%$

[a] Standard deviation as computed from the difference between the value of an experimental result (as tabulated in the appendix) and that from the smooth functions reported above.

TABLE 4. *Results on properties of hafnium–3 (wt. %) zirconium*

Phase	T (K)	c_p (J·g^{-1}·K^{-1})	ρ (10^{-8}Ω·m)
α	1500	0.2006	158.94
	1600	.2044	161.60
	1700	.2082	163.67
	1800	.2120	165.14
	1900	——	166.00
	2000	——	166.27
β	2100	——	154.15
	2200	0.1974	155.28
	2300	.2025	156.41
	2400	.2090	157.53

TABLE 5. *Error analysis*

Quantity	Imprecision[a]	Inaccuracy[b]
Temperature (at 2000 K).....	0.5K	4K
Voltage.....	.03%	0.1%
Current.....	.03%	0.1%
Specific heat.....	.5	3%
Electrical resistivity.....	.2	1%
Hemispherical total emittance.....	——	5%

[a] Imprecision refers to the standard deviation of a quantity as computed from the difference between the value of the quantity and that from the smooth function obtained by the least squares method. The quantities in the case of temperature, voltage, and current are the individual points measured in a single experiment, and in the case of specific heat and electrical resistivity are the results from all experiments as tabulated in the appendix.

[b] Inaccuracy refers to the estimated total error (random and systematic).

3. Discussion

The specific heat and electrical resistivity of hafnium–3 (wt. %) zirconium measured in this work are presented in figures 1 and 2, respectively, and are compared graphically with the results reported in the literature on hafnium containing varying amounts of zirconium. The results reported in the literature were for temperatures below 2200 K. In this work, the measurements were extended to 2400 K, which is approximately 100 K below the melting point of hafnium.

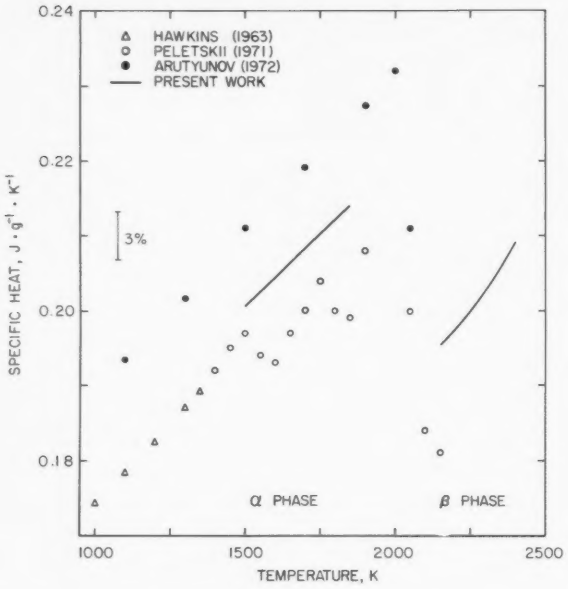

FIGURE 1. *Specific heat of hafnium reported in the literature.*

Zirconium content in weight percent is: 2.8, Hawkins et al [7]; 0.66. Peletskii and Druzhinin [6]; 0.65, Arutyunov et al [5]; and 3.12 present work.

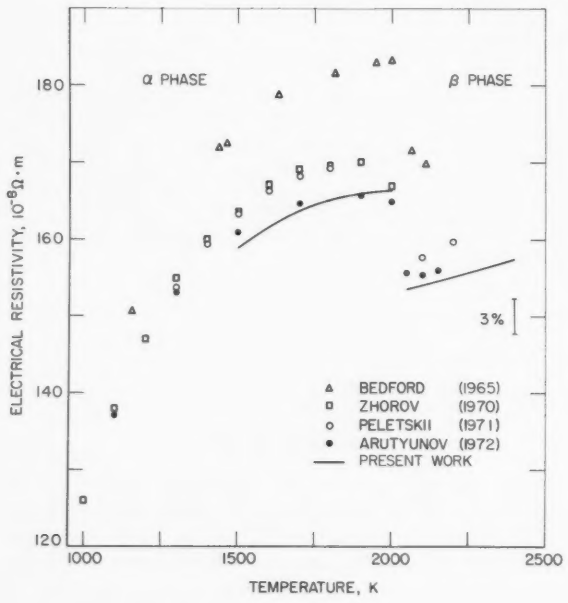

FIGURE 2. *Electrical resistivity of hafnium reported in the literature.*

Zirconium content in weight percent is: 2.4, Bedford [9]; 0.96, Zhorov [8]; 0.66, Peletskii and Druzhinin [6]; 0.65 Arutyunov et al [5]; and 3.12 present work.

3.1. Specific Heat

Zirconium content (2.8 wt. %) of the specimen used by Hawkins et al. [7] was comparable to that of the specimen used in the present work. Extrapolation of the results of Hawkins et al. from 1350 K to 1500 K yields a value which is approximately 2.5 percent lower than the present work result. Arutyunov et al. [5] and Peletskii and Druzhinin [6] have reported measurements using specimens with lower zirconium content–approximately 0.65 (wt. %) zirconium. However, their results are in considerable disagreement with each other (6 to 10 %). The results (after correcting for zirconium content) of the present work are about 5 percent lower than those of Arutyunov et al., and on the average about 4 percent higher than those of Peletskii and Druzhinin in the overlaping temperature regions below the transformation point. Above the transformation point, only a few measurements (all below 2200 K) were reported by the above investigators. Because of the insufficient data, it was not possible for them to establish the trend of specific heat versus temperature in the range between the transformation and the melting points.

The results of the present work indicate the following trend for specific heat as a function of temperature: (1) before transformation–increases nearly linearly, (2) at the transformation point–decreases sharply, and (3) above the transformation point–increases with an increasing rate of change. Extrapolation of the results to the transformation temperature, 2012 K [10], indicates a change in specific heat of 12.9 percent[2] (0.0283 $J \cdot g^{-1} \cdot K^{-1}$) during the transformation. A similar procedure applied to the results reported in the literature yields the following approximate values for the change in specific heat during transformation: 13.0 percent (Peletskii and Druzhinin [6]) and 9.1 percent (Arutyunov et al. [5]). The latter is likely to be low since data did not extend beyond the initial transformation period.

Table 6 gives estimated results of the heat capacity of pure hafnium obtained from the present work data after making a correction for the zirconium content

TABLE 6. *Heat capacity of pure hafnium*

Phase	Temperature (K)	Heat capacity ($J \cdot mol^{-1} \cdot K^{-1}$)
α	1500	35.0
	1600	35.7
	1700	36.4
	1800	37.0
β	2200	34.1
	2300	35.0
	2400	36.3

[2] Computed according to the relation:

$$\Delta c_p = 100[(c_p)_{\text{before}} - (c_p)_{\text{after}}]/(c_p)_{\text{before}}.$$

(using Kopp's additivity law). Heat capacity of zirconium needed for this correction is obtained from an earlier publication [11]. The atomic weight of hafnium was taken as 178.49 [13]. It may be seen that at 2400 K (about 100 K below its melting point), heat capacity of hafnium reaches a value of 36.3 $J \cdot mol^{-1}K^{-1}$, which is considerably higher than the Dulong and Petit value of $3R$ (24.943 $J \cdot mol^{-1} \cdot K^{-1}$).

3.2. Electrical Resistivity

Electrical resistivity results for hafnium reported in the recent literature [5, 6, 8, 9], with one exception [9], are in agreement with those of the present work within 3 percent. The results of Bedford [9] are 5 to 10 percent higher than those of the other investigators. This difference cannot be attributed to the high value of zirconium content in the specimen (about 2.4 percent by weight), since the present work results, which were obtained on specimens of comparable composition, were lower than those of the other investigators. The zirconium content of specimens used by Arutyunov et al. [5] and Peletskii and Druzhinin [6] was about 0.65 percent by weight, while the specimen used by Zhorov [8] contained about 1 percent zirconium. The results of all the investigators show a decrease in electrical resistivity as the result of the $\alpha \rightarrow \beta$ transformation. However, because of the insufficient data, it was not possible to establish the trend of resistivity versus temperature in the range between the transformation and the melting points.

The results of the present work indicate the following trend for electrical resistivity as a function of temperature: (1) before transformation increases with a decreasing rate of change, (2) during transformation decreases sharply, and (3) after transformation increases with an increasing rate of change. Extrapolation of the results to the transformation temperature [3] indicate a change in electrical resistivity of 7.9 percent ($13.1 \times 10^{-8} \Omega \cdot m$) during the transformation. The data reported in the literature yield the following results for the change in electrical resistivity during the transformation: 6.4 percent (Arutyunov et al. [5]), 6.9 percent (Peletskii and Druzhinin [6]), and 7.3 percent (Bedford [9]). Zhorov's measurements did not extend beyond the initial transformation period, thus it was not possible to obtain a meaningful result on resistivity change. Earlier measurements by Fast [12] of the resistance change in a hafnium specimen containing 3 weight percent zirconium during transformation yielded a value of 7.5 percent.

A distinct advantage of the method employed in this work is that it provides resistivity data during the entire transformation period. This allows the accurate determination of the variation of electrical resistivity as a function of time and temperature near and at the transformation point. The results of a typical experiment are shown in figures 3 and 4.

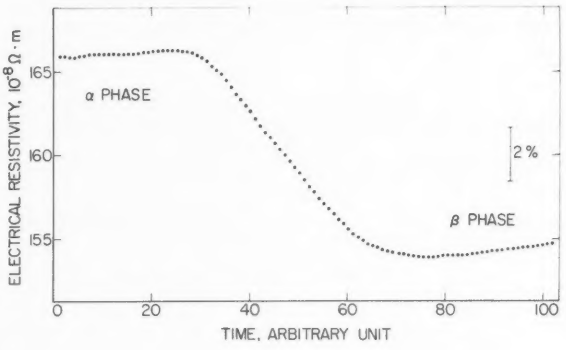

FIGURE 3. *Variation of electrical resistivity as a function of time near and at the $\alpha \rightarrow \beta$ transformation point of hafnium-3 (wt %) zirconium.*

(The curve refers to specimen 1; 1 time unit = 0.833 ms).

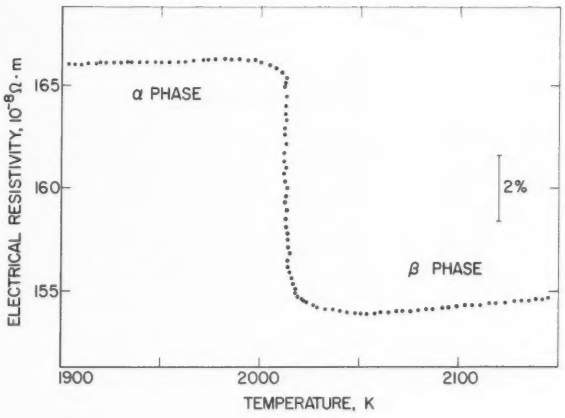

FIGURE 4. *Variation of electrical resistivity as a function of temperature near and at the $\alpha \rightarrow \beta$ transformation point of hafnium-3 (wt %) zirconium.*

(The curve refers to specimen 1).

[3] Computed according to the relation:

$$\Delta\rho = 100\ (\rho_{\text{before}} - \rho_{\text{after}})/\rho_{\text{before}}$$

3.3. Hemispherical Total Emittance

Hemispherical total emittance was measured at three temperatures, two below and one above the transformation point. A comparison of the present work results with those reported in the literature (table 7) shows a general agreement in the range 0 to 5 percent at temperatures 1700 and 1870 K. No data was located in the literature for temperatures above 2200 K. From the available data no satisfactory conclusion could be drawn regarding the effect of zirconium on the hemispherical total emittance of hafnium.

TABLE 7. *Hemispherical total emittance of hafnium containing various amounts of zirconium as reported in the literature*

Investigator	Ref.	Zirconium content (wt. %)	Temperature, K		
			1700	1870	2280
Zhorov	[8]	0.96	0.330	0.330	—
Peletskii and Druzhinin	[6]	0.66	.306	.316	—
Arutyunov et al.	[5]	0.65	.312	.323	—
Present work		3.12	.320	.330	0.342

4. Appendix

TABLE A-1. *Experimental results on specific heat of hafnium-3 (wt %) zirconium*[a]

Phase	Temp. (K)	Specimen-1				Specimen-2	
		First heating		Second heating			
		c_p	Δc_p	c_p	Δc_p	c_p	Δc_p
α	1500	0.2012	+0.32	0.2008	+0.12	0.2002	−0.17
	1550	0.2022	−0.13	0.2031	+0.31	0.2019	−0.28
	1600	0.2044	+0.01	0.2053	+0.45	0.2042	−0.09
	1650	0.2062	−0.04	0.2066	+0.15	0.2060	−0.14
	1700	0.2079	−0.15	0.2080	−0.10	0.2076	−0.29
	1750	0.2097	−0.20	0.2097	−0.20	0.2097	−0.20
	1800	0.2117	−0.16	0.2117	−0.16	0.2123	+0.12
	1850	0.2140	+0.02	0.2142	+0.12	0.2154	+0.67
β	2150	0.1952	−0.13	0.1956	+0.07	0.1950	−0.24
	2200	0.1976	+0.07	0.1975	+0.02	0.1978	+0.18
	2250	0.2002	+0.20	0.1993	−0.26	0.2007	+0.44
	2300	0.2028	+0.13	0.2012	−0.66	0.2038	+0.62
	2350	—	—	0.2037	−0.94	0.2055	−0.06
	2400	—	—	0.2079	−0.56	0.2113	+1.06

[a] Specific heat is in $J \cdot g^{-1} \cdot K^{-1}$, and the quantity Δc_p is percentage deviation of the individual results from the smooth functions represented by the pertinent eqs in table 3.

TABLE A-2. *Experimental results on electrical resistivity of hafnium-3 (wt. %) zirconium* [a]

Phase	Temp. (K)	Specimen-1				Specimen-2	
		First heating		Second heating			
		ρ	$\Delta\rho$	ρ	$\Delta\rho$	ρ	$\Delta\rho$
α	1500	158.97	+0.02	159.52	+0.36	157.94	−0.63
	1550	160.54	+0.12	160.96	+0.38	159.61	−0.46
	1600	161.85	+0.15	162.15	+0.33	161.02	−0.36
	1650	163.02	+0.18	163.21	+0.30	162.39	−0.20
	1700	163.92	+0.15	164.02	+0.21	163.35	−0.20
	1750	164.65	+0.10	164.66	+0.11	164.15	−0.20
	1800	165.23	+0.04	165.16	+0.01	164.79	−0.21
	1850	165.65	0.00	165.54	−0.07	165.28	−0.22
	1900	166.10	+0.05	165.94	−0.04	165.82	−0.11
	1950	166.36	+0.08	166.14	−0.05	166.09	−0.08
	2000	166.57	+0.17	166.30	+0.01	166.37	+0.06
β	2050	153.93	+0.22	—	—	153.33	−0.17
	2100	154.34	+0.12	154.53	+0.25	153.68	−0.30
	2150	154.83	+0.08	154.83	+0.08	154.26	−0.29
	2200	155.44	+0.10	155.42	+0.09	154.87	−0.26
	2250	156.01	+0.11	156.02	+0.12	155.49	−0.22
	2300	156.55	+0.09	156.63	+0.14	156.13	−0.18
	2350	—	—	157.26	+0.08	156.70	−0.17
	2400	—	—	157.76	+0.14	157.30	−0.15

[a] Electrical resistivity is in $10^{-8}\Omega \cdot m$, and the quantity $\Delta\rho$ is percentage deviation of the individual results from the smooth functions represented by the pertinent eqs in table 3.

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Paper 79A2–850

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Heat Capacities of Polyethylene III. One Linear and One Branched Sample from 5 to 350 K

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Heat capacities of two polyethylene samples, one linear with a density of 0.973 g cm^{-3} and one branched with a density of 0.91 g cm^{-3}, have been determined by adiabatic calorimetry from 5 to 360 K in a different experimental arrangement then employed for studies of other polyethylene samples in this series. The heat capacity behavior of these two samples confirms expectations for samples with corresponding densities.

Key words: Adiabatic calorimetry; branched polyethylene; calorimetry; cryogenic temperature; heat capacity; linear polyethylene; polyethylene; thermodynamic properties.

1. Introduction

Heat capacities of two polyethylene samples, one linear and one branched, were determined from 5 to 350 K by adiabatic calorimetry. The linear sample has been treated to yield a relatively high density value of 0.973 g cm^{-3}. The branched sample was one of the lowest density polyethylene sample available, its density value is 0.91 g cm^{-3}. The heat capacity behavior of these two samples, produced by different sources and measured with different experimental arrangements than that for four samples derived from two Standard Reference Materials [1, 2],[1] closely parallels the behavior (as a function of density) of the Standard Reference Materials [2].

2. Experimental Detail

2.1. Calorimetry

Heat capacities of the two polyethylene samples were measured with the Mark I cryostat in the Department of Chemistry, University of Michigan, Ann Arbor, Michigan. The design and the operational procedures of this aneroid-type adiabatic cryostat have been described elsewhere [3, 4], and are similar to a cryostat described in more detail elsewhere [5]. The gold-plated copper sample container, laboratory designation W–9 [6], was used in the measurements of the branched polyethylene sample. Container, W–10, was used in the measurements of the linear polyethylene sample. Container W–10 is of similar design to W–9 except that there are no internal vanes for thermal conduction and the entire top of the container is made of copper and is removable for the admission of samples.

Temperatures were measured by a capsule-type platinum resistance thermometer, laboratory designation A–3, inserted in the axial well of the sample container. This thermometer has been calibrated by the National Bureau of Standards (NBS) according to the International Practical Temperature Scale (IPTS) of 1948 above 90 K; and to the NBS–1955 provisional temperature scale between 10 and 90 K. Below 10 K, a laboratory provisional scale was obtained by solving for the constants in the equation [7] $R = A + BT^2 + CT^5$ from the observed resistances at the boiling point of helium and at 10 K and the dR/dT value at 10 K.

To correct the original heat capacity data to temperatures expressed in terms of IPTS–1968 [8], the following procedures were used to provide adjustments between the several temperature scales.

Above 13.81 K, an approximate correction scheme was used to correct the heat capacities to values they

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[1] Figures in brackets indicate the literature references at the end of this paper.

would have if they were determined by a thermometer calibrated in accordance to the IPTS–1968 [8]. This procedure [9] involves the multiplication of each experimental heat capacity value by a factor of $1 + d(T_{68} - T)/dT$, where T is the temperature scale used in the experiment and $(T_{68} - T)$ is the difference between the IPTS–1968 and the experimental temperature scale. Tables of the differences between the IPTS–1968 and the IPTS–1948 or the NBS–1955 provisional scale are given in reference [10], and in more detail elsewhere [11].

Heat capacity values below 13.81 K may be corrected from the previously mentioned laboratory provisional temperature scale to a temperature scale which approximates the thermodynamic temperature scale or the NBS–1965 (2–20 K) temperature scale [12] based on acoustic thermometry. An improved thermometer calibration with an accuracy of about 0.02 K was obtained from a two-way structure analysis of the behaviors of a group of platinum resistance thermometers [13]. The differences between this improved calibration and the laboratory provisional scale were then used to correct the heat capacity values in a manner similar to the procedure described above for correcting heat capacity values at temperatures above 13.81 K.

2.2. Materials

a. Linear Polyethylene

A molded piece of Marlex 50[2] was supplied by Dr. Raymond L. Arnett of the Phillips Petroleum Co., Bartlesville, Oklahoma. This piece was machined as a cylinder with an axial hole (to accommodate the thermometer-heater wall) and was then loaded into the sample container, laboratory designation W–10, which has no thermal conducting vanes. The density of the machined sample was determined to be 0.973 g cm^{-3}. The mass of the calorimetric sample was 87.121 g in vacuo. Helium gas at a pressure of 815 mm Hg (108 kPa) was sealed in to aid the thermal conduction within the sample container. Indium-tin alloy (50–50) was used to seal the top of the sample container. Apiezon.T grease was used to establish thermal contact between the sample container and the heater-thermometer assembly. In order to minimize the corrections, masses of both solder and grease were adjusted to approximately the values used when the heat capacity of the empty sample container was measured.

b. Branched Polyethylene

A sample with the designation DYNH CT–1660 was also supplied by Dr. Raymond L. Arnett of the Phillips Petroleum Co., Bartlesville, Oklahoma. This sample consists of cylindrical pellets about 5 mm diam and 5 mm length. The density was reported by Dr. Arnett to be 0.91 g cm^{-3}. A sample mass of 45.122 g in vacuum was loaded in the sample container, laboratory designation W–9. Dried and purified helium gas at a pressure of 190 mm Hg (25.2 kPa) was sealed in the calorimeter to aid the thermal conduction. Masses of indium-tin (50–50) solder and grease are adjusted to approximate the amounts used during empty sample container measurements.

[2]Certain commercial equipment, instruments, or materials are identified in this paper in order to adequately specify the experimental procedure. In no case does such identification imply recommendation or endorsement by the National Bureau of Standards, nor does it imply that the material or equipment identified is necessarily the best available for the purpose.

3. Results

The experimental heat capacity determinations are listed chronologically in table 1 and are shown graphically in Figure 1. The approximate temperature increments of each determination may be inferred from the adjacent mean temperatures in a series of continuous determinations. An analytically determined curvature correction has been applied to the observed values of $\Delta H/\Delta T$ to correct for the finite size of the temperature increment used in the heat capacity determination. The molecular weight for the repeating methylene segment, —CH_2—, is taken as 14.027. Molal values of the heat capacity at constant pressure and the entropy and enthalpy increments generated by a least-square curve-fitting program are listed at selected rounded temperatures in table 2. The reported values of the heat capacities are believed to have probable errors less than 0.1 percent at temperatures above 25 K, about 1 percent at 10 K and 5 percent at 5 K. The probable error of the thermodynamic functions are considered to be less than 0.1 percent above 100 K. H_0 and S_0 refer to the zero point enthalpy

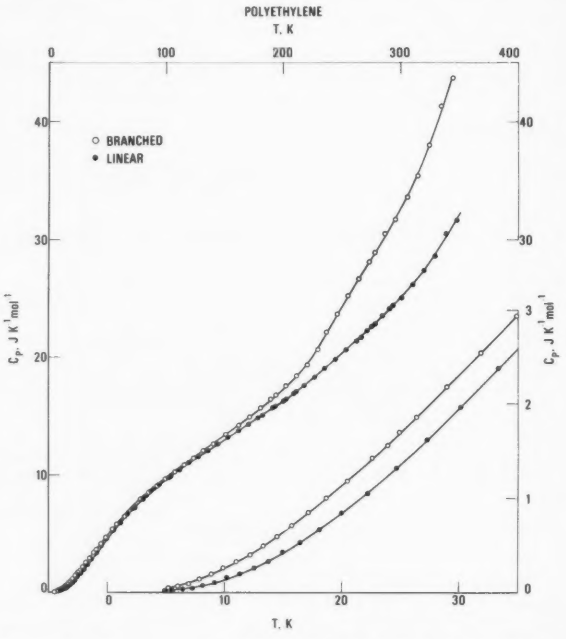

FIGURE 1. *Heat capacities of 1 linear and 1 branched polyethylene samples.*

●– Marlex 50, ○– DYNH CT–1660.

and residual entropy of individual samples. Gibbs energies for these samples are not given in table 2, because these samples are expected to have undetermined residual entropies at 0 K.

TABLE 1. *Heat Capacities of Polyethylene*

(base mole $[-CH_2-]=14.027$)

A. Linear Polyethylene ($\rho=0.973$ g cm^{-3})

T, K	C_p, J K^{-1} mol^{-1}
SERIES I	
80.41	7.953
83.41	8.242
89.78	8.841
SERIES II	
104.13	9.856
111.84	10.41
119.96	11.07
128.03	11.51
136.03	12.09
144.31	12.64
152.99	13.21
161.82	13.78
170.27	14.32
178.43	14.83
SERIES III	
182.55	15.07
191.25	15.65
200.25	16.26
209.09	16.86
217.87	17.51
226.96	18.20
SERIES IV	
235.53	18.99
244.50	19.75
253.69	20.51
262.73	21.34
271.59	22.17
SERIES V	
275.83	22.58
284.92	23.48
293.96	24.40
SERIES VI	
291.67	24.10
300.82	25.09
310.33	26.18
320.12	27.36
329.53	28.58
338.51	30.46
347.51	31.62
SERIES VII	
4.83	0.016
5.58	0.022
6.44	0.035
7.25	0.054
8.16	0.081
9.15	0.122
10.21	0.176
11.31	0.210
12.52	0.265
13.77	0.341
15.06	0.429
16.48	0.533
18.15	0.667
20.07	0.841
22.25	1.055
24.69	1.317
27.30	1.622
30.15	1.964
33.34	2.375
36.90	2.845
40.89	3.376
45.23	3.945
49.84	4.542
SERIES VIII	
50.12	4.574
55.46	5.236
61.16	5.935
67.26	6.620
73.65	7.214
80.32	7.934
87.05	8.613
94.22	9.144
102.37	9.734
SERIES IX	
193.27	15.80
202.14	16.36
211.13	16.99
SERIES X	
266.77	21.63
278.40	22.75

TABLE 1—Continued

B. Branched Polyethylene ($\rho=0.91$ g cm^{-3})

T, K	C_p, J K^{-1} mol^{-1}
SERIES I	
5.20	0.039
6.05	.062
6.98	.098
7.87	.146
8.87	.200
9.90	.284
11.04	.331
12.20	.406
13.32	.499
14.51	.597
15.79	.712
17.16	.841
18.70	.997
20.52	1.184
22.63	1.422
24.93	1.708
SERIES II	
23.94	1.563
26.39	1.858
29.00	2.175
31.87	2.540
34.93	2.931
38.47	3.381
SERIES III	
40.32	3.612
44.44	4.125
48.95	4.681
54.26	5.306
SERIES IV	
58.16	5.749
64.59	6.473
71.56	7.331
78.46	7.661
85.47	8.506
92.32	9.068
99.62	9.621
107.66	10.23
115.56	10.83
123.49	11.42
131.71	12.03
151.04	13.45
161.99	14.22
171.15	14.93
180.32	15.66
189.54	16.39
SERIES V	
193.89	16.74
202.65	17.54
211.45	18.38
220.45	19.35
229.57	20.60
SERIES VI	
237.06	22.08
246.25	23.64
255.39	25.18
264.61	26.60
273.75	28.08
SERIES VII	
278.37	28.92
286.74	30.43
295.89	31.67
305.57	33.52
314.85	35.34
SERIES VIII	
324.45	37.97
334.68	41.29
344.69	43.72

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TABLE 2. *Thermodynamic Properties of Polyethylene*

(Units in K, J and mole [—CH_2—]=14.027)

T	Linear (Marlex 50)			Branched (DYNH CT–1660)		
	C_p	$H-H_0$	$S-S_0$	C_p	$H-H_0$	$S-S_0$
5	0.020	0.03	0.007	0.038	0.05	0.013
10	0.155	0.38	0.050	0.273	0.72	0.097
15	0.422	1.77	0.160	0.636	2.94	0.272
20	0.833	4.85	0.334	1.134	7.32	0.521
25	1.357	10.29	0.574	1.696	14.39	0.833
30	1.941	18.51	0.872	2.303	24.36	1.195
35	2.595	29.84	1.221	2.944	37.48	1.599
40	3.254	44.46	1.610	3.570	53.77	2.033
45	3.911	62.38	2.031	4.187	73.16	2.489
50	4.557	83.55	2.477	4.798	95.63	2.962
60	5.789	135.4	3.418	5.988	149.6	3.943
70	6.912	199.0	4.396	7.092	215.1	4.950
80	7.915	273.2	5.386	8.063	291.0	5.962
90	8.801	356.9	6.371	8.901	375.9	6.961
100	9.592	448.9	7.340	9.651	468.7	7.938
110	10.31	548.5	8.288	10.39	568.9	8.893
120	11.00	655.1	9.215	11.17	676.7	9.830
130	11.67	768.4	10.12	11.92	792.2	10.75
140	12.36	888.5	11.01	12.62	914.8	11.66
150	13.02	1016	11.89	13.36	1045	12.56
160	13.67	1149	12.75	14.11	1182	13.45
170	14.30	1289	13.60	14.85	1327	14.32
180	14.93	1435	14.43	15.62	1479	15.19
190	15.57	1587	15.26	16.41	1639	16.06
200	16.23	1746	16.07	17.27	1808	16.92
210	16.93	1912	16.88	18.24	1985	17.79
220	17.67	2085	17.68	19.37	2173	18.66
230	18.48	2266	18.49	20.75	2373	19.55
240	19.35	2455	19.29	22.59	2590	20.47
250	20.23	2653	20.10	24.32	2825	21.43
260	21.11	2859	20.91	25.93	3076	22.42
270	22.00	3075	21.72	27.50	3343	23.42
280	22.93	3300	22.54	29.08	3626	24.45
290	23.92	3534	23.36	30.75	3925	25.50
300	24.99	3778	24.19	32.55	4241	26.57
310	26.15	4034	25.03	34.56	4577	27.67
320	27.43	4302	25.88	36.83	4933	28.81
330	28.84	4583	26.74	39.43	5314	29.98
340	30.41	4879	27.63	42.42	5723	31.20
350	32.16	5192	28.53	45.87	6164	32.48
273.15	22.29	3145	21.98	27.99	3430	23.75
298.15	24.79	3732	24.04	32.20	4181	26.37

In the course of determining the heat capacities of the linear polyethylene sample from Series I to IV, there was a loose connection in the circuit for the heater current measurement. Therefore, the energy input was calculated by adjusting the observed heater resistance values to the known resistance values obtained from previous measurements. These corrections ranged from 1 to 3 percent of the observed heat capacity values. After series IV, it was found that the top of the sample container was pushed out, apparently due to the large thermal expansion of the sample at higher temperatures. The measurements starting from Series V were made after the sample container top was resoldered and the container was sealed in with helium gas at a pressure of 719 mm (95.5 kPa).

The heat capacity of the calorimetric sample of Marlex 50 is about 2–3 percent lower than that of SRM–1475 in the as received condition [1]. The differences are probably due to the difference in the densities and the degrees of crystallinity of the two samples. The density of SRM 1475 as received is 0.955 g cm^{-3}, which is slightly lower than that of the Marlex 50 sample, 0.971 g cm^{-3}, used in the present calorimetric study. The higher density indicates a higher crystalline content or a lower amorphous content. The heat capacity of crystalline polyethylene is lower than that of the amorphous phase over the entire temperature range of investigation. Below 300 K, the behavior of the present linear polyethylene sample agrees very well with the values obtained by interpolating to the corresponding density from the behaviors of three linear polyethylene samples of the same origin but of different densities in figure 2 of reference [2].

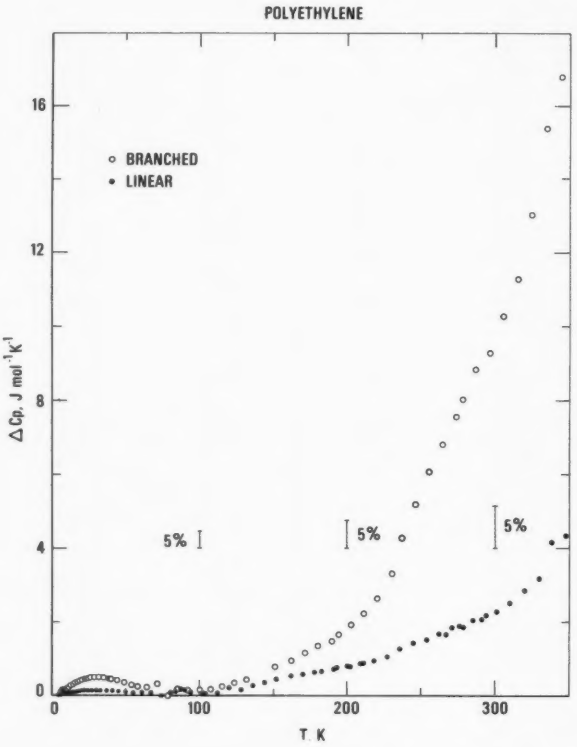

FIGURE 2. *Comparison of heat capacities of polyethylene samples versus estimated heat capacity of crystalline linear polyethylene.*

●—linear, Marlex 50, ○—branched, DYNH CT–1660.

When the heat capacity differences between the Marlex 50 and estimated completely crystalline linear polyethylene [2] are plotted in Figure 2, two regions of more abrupt rise in the heat capacity differences, around 150 and 250 K, may be noticed. The higher temperature rise has been ascribed to the glass transition phenomena on the basis of adiabatic temperature drift observations [14] and volume relaxation studies [15]. Heat capacity values for Marlex 50 based on IPTS–1948 and NBS–1955 scales were used in the difference plots in figure 7 of reference

[2]. After the values have been corrected to IPTS–1968 representation as described in previous section, the irregularities in the region 70–90 K due to the joining of the two scales [16] are diminished in magnitude but still noticeable.

The heat capacity behavior of the branched polyethylene used in this study is very similar to that of SRM–1476 branched polyethylene whole polymer [1]. Except in the region from 100 to 200 K, the heat capacities of these two samples and other branched polyethylene samples [17, 18, 19] are in general slightly higher than linear polyethylene results extrapolated to corresponding densities (cf. fig. 2 in reference [2]). Thus, the curves of the difference between the heat capacities, figure 2, of the branched polyethylene and 100 percent crystalline linear polyethylene show a more pronounced abrupt change in the region of 250 K than the corresponding curves for linear polyethylene and almost smooth curves in the region of 150 K.

Relatively large positive temperature drifts have been observed during the measurements of the branched polyethylene DYNH CT–1660 sample. In the 200 to 300 K region, a maximum drift of 0.01 K min^{-1} was observed at around 255 K. This is probably similar to that which has been observed for the quenched, branched polyethylene, SRM 1476, in reference [1]. At temperatures above 300 K, the drift of DYNH CT–1660 gradually increased to about 0.15 K min^{-1} at about 350 K. Similar behavior has been noted for SRM–1476 when it was heated above room temperature for the first time [1]. Calorimetric temperature drifts longer and larger than usual have also been observed for the linear polyethylene, Marlex 50, sample at temperatures above 220 K. Below 300 K, the maximum temperature drift observed at 30 min after the termination of heater input was less than 0.005 K min^{-1}. Near the highest measurement temperature the drift was still less than 0.01 K min^{-1}.

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Publications of the National Bureau of Standards*

Citations with Selected Abstracts

J. Res. Nat. Bur. Stand. (U.S.), **79A** *(Phys. and Chem.)*, No. 1 (Jan.-Feb. 1975), SD Catalog No. C13.22/sec.A:79/1.

Polarization effects on fluorescence measurements, E. D. Cehelnik, K. D. Mielenz, and R. A. Velapoldi.

The iron-neon hollow-cathode spectrum, H. M. Crosswhite.

Equation of state for themodynamic properties of fluids, R. D. Goodwin.

Thermodynamic studies of the $\alpha \rightarrow \beta$ phase transformation in zirconium using a subsecond pulse heating technique, A. Cezairliyan and F. Righini.

SP260-49. **Standard reference materials: Calibrated glass standards for fission track use,** B. S. Carpenter and G. M. Reimer, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-49, 25 pages (Nov. 1974) SD Catalog No. C13.10:260-49, 75 cents.

Key words: fission tracks; flux monitors; glass standards; standard reference material; thermal neutron irradiation; uranium.

Four glasses of different uranium concentrations were prepared and certified by the National Bureau of Standards as standards for use as neutron monitors to aid fission track studies. These Standard Reference Materials (SRM) and their uranium concentrations are: SRM 941 (461 ppm), SRM 962 (37.4 ppm), SRM 963 (0.823 ppm), and SRM 964 (0.0721 ppm). These glass wafers were irradiated in the National Bureau of Standards Reactor and the neutron flux was monitored using copper and gold foils.

SP396-1. **Critical surveys of data sources: Mechanical properties of metals,** R. B. Gavert, R. L. Moore, and J. H. Westbrook, Nat. Bur. Stand. (U.S.), Spec. Publ. 396-1, 90 pages (Sept. 1974) SD Catalog No. C13.10:396-1, $1.25.

Key words: commercial alloys; data sources; mechanical properties; metals.

This study was undertaken with the objective of providing a detailed critical survey of the existent sources of mechanical property data for commercially available metals and alloys. This survey was intended to assess the scope, assets and deficiencies of about forty of the most prominent sources of such information. There were included: handbooks and technical compilations, information centers, foreign information sources, technical societies, and trade associations. The initial listing of sources to be examined was prepared by the authors with the advice and the assistance of a subcommittee of the Metals Properties Council. The aim was to restrict the survey to sources which actually had compilations of mechanical property data in some form. Thus sources which offered only generalized guides to the literature, monographs, textbooks, or periodicals publishing original research or engineering articles were not to be included. Those sources from the original listing which were found upon detailed examination to fall into the latter categories are therefore treated in a separate appendix.

SP398. **Fundamental physical constants,** B. N. Taylor, Nat. Bur. Stand. (U.S.), Spec. Publ. 398, pocket card (Aug. 1974) SD Catalog No. C13.10:398, 25 cents.

Key words: fundamental constants.

This card gives values of the fundamental constants resulting from the "1973 Least-Squares Adjustment of the Fundamental Physical Constants" carried out by E. R. Cohen and B. N. Taylor under the auspices of the CODATA Task Group on Fundamental Constants and adopted for international use by CODATA. These constants have been previously given in J. Phys. Chem. Ref. Data **2**, 663 (1973) and CODATA Bulletin No. 11 (Dec. 1973). Supersedes NBS SP344.

SP399. Volume 1. **NBS FORTRAN test programs. Volume 1—documentation for versions 1 and 3,** F. E. Holberton and E. G. Parker, Nat. Bur. Stand. (U.S.), Spec. Publ. 399, 171 pages (Oct. 1974) SD Catalog No. C13.10:399/V.1, $2.35.

Key words: computer programming language; FORTRAN; FORTRAN validation; language validation; standard FORTRAN; test program design.

The NBS FORTRAN test programs, written in Standard FORTRAN, are designed to test whether a FORTRAN compiler accepts the forms and interpretations of the FORTRAN language as described in the American National Standard FORTRAN document X3.9-1966. The test programs, comprised of 116 test units, are structured into two versions, each containing approximately 14,500 punch card images. The test units may be used as separate executable FORTRAN programs, or may be linked end to end with other test units, with a minimum of user effort, to improve operating efficiency. Version 1 is structured into 116 executable FORTRAN programs, and Version 3, containing the same 116 test units, is structured into 14 executable FORTRAN programs for use on large FORTRAN processors.

The test program design criteria was to: Constrain all test programs to the FORTRAN Standard X3.9-1966; Reduce the effect of those areas in which the FORTRAN Standard does not prescribe a method or sulution, e.g., range, precision, size of computer, etc.; Simplify the use of the FORTRAN test programs; Test FORTRAN language elements before they are used in support of other tests; Maintain an open ended system so that tests may be changed or added.

The test programs require the use of a card reader, printer and one intermediate tape unit.

SP399. Volume 2. **NBS FORTRAN test programs. Volume 2—listings for version 1,** F. E. Holberton and E. G. Parker, Nat. Bur. Stand. (U.S.), Spec. Publ. 399, 221 pages (Oct. 1974) SD Catalog No. C13.10:399/V.2, $2.85.

**Publications with prices and SD Catalog numbers may be purchased directly from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402 (foreign: one-fourth additional). Microfiche copies of the above, plus paper copy and microfiche versions of NBS Interagency Reports (NBSIR's), may be purchased from the National Technical Information Service (NTIS), Springfield, Va. 22161. Prices are subject to change. Reprints from the NBS Journal of Research and non-NBS publications may often be obtained directly from the authors.*

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The test programs require the use of a card reader, printer and one intermediate tape unit.

SP399. Volume 3. **NBS FORTRAN test programs. Volume 3 – listings for version 3,** F. E. Holberton and E. G. Parker, Nat. Bur. Stand. (U.S.), Spec. Publ. 399, 226 pages (Oct. 1974) SD Catalog No. C13.10:399/V.3, $2.90.

Key words: computer programming language; FORTRAN; FORTRAN validation; language validation; standard FORTRAN; test program design.

The NBS FORTRAN test programs, written in Standard FORTRAN are designed to test whether a FORTRAN compiler accepts the forms and interpretations of the FORTRAN language as described in the American National Standard FORTRAN document X.3.9-1966. The test programs, comprised of 116 test units, are structured into two versions, each containing approximately 14,500 punch card images. The test units may be used as separate executable FORTRAN programs, or may be linked end to end with other test units, with a minimum of user effort, to improve operating efficiency. Version 1 is structured into 116 executable FORTRAN programs, and Version 3, containing the same 116 test units, is structured into 14 executable FORTRAN programs for use on large FORTRAN processors.

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The test programs require the use of a card reader, printer and one intermediate tape unit.

SP400-4. **Semiconductor measurement technology. Combined quarterly report, October 1, 1973 to March 31, 1974,** W. Bullis, Ed., Nat. Bur. Stand. (U.S.), Spec. Publ. 400-4, 101 pages (Nov. 1974) SD Catalog No. C13.10:400-4, $1.70.

Key words: boron redistribution; collector resistor; doping profiles; effective masses; electrical properties; electron beam induced current mode electronics; epitaxial layer thickness; flying spot scanner; gold-doped silicon; hermeticity; ion microprobe mass analysis; methods of measurement; microelectronics; microwave diodes; mobility; MOS devices; oxide films; photomasks; photoresist; platinum wire resistivity; resistivity standards; ribbon wire scanning electron microscopy; semiconductor devices; semiconductor materials; semiconductor process control; sheet resistance; silicon; spreading resistance; test patterns; thermal response; thermally stimulated capacitance; thermally stimulated current; thick film copper; voltage contrast mode; wire bonds; x-ray photoelectron spectroscopy.

This combined quarterly progress report describes NBS activities directed toward the development of methods of measurement for semiconductor materials, process control, and devices. Principal accomplishments during this reporting period include (1) identification of major problem areas in connection with measuring and inspecting photomasks, (2) development of a mathematical model suitable for interpreting thermally stimulated current and capacitance measurements on junction diodes and metal-oxide-semiconductor (MOS) capacitors, (3) completion of a preliminary evaluation of a method, based on the transient capacitance-voltage characteristic of an MOS capacitor, for measuring thickness of epitaxial layers up to 2 μm, and (4) development of criteria for use in nondestructive wire bond pull tests. Results are also reported on spreading resistance, capacitance-voltage, and carrier mobility measurements; polynomial fits for energy band gap and hole and electron effective masses in silicon; methods for characterizing oxide films; evaluation of sheet resistance and collector resistor test structures; evaluation of a photoresist spinner test; scanning electron microscopy; bonding of aluminum ribbon wire to thick film copper; bonding of platinum wire to thin film aluminum; leak rate calculations in the transition flow regime; transistor thermal response measurements; and radiation response of microwave mixer diodes. Supplementary data concerning staff, publications, workshops and symposia, standards committee activities, and technical services are also included as appendices.

SP400-9. **Semiconductor measurement technology: ARPA/NBS Workshop II. Hermeticity testing for integrated circuits,** H. A. Schafft, Nat. Bur. Stand. (U.S.), Spec. Publ. 400-9, 43 pages (Dec. 1974) SD Catalog No. C13.10:400-9, $1.00.

Key words: bubble test; gas analysis; helium leak test; hermeticity; integrated circuits; measurement methods; microelectronics; radioisotope test; seals; semiconductor devices; weight test.

Synopses are presented of the six invited talks and two discussion periods of a meeting in which 65 engineers and scientists, representing 36 organizations from private industry and government, participated. Topics ranged from failure analysis and the nature of leaks to evaluations and intercomparisons of bubble, weight, helium, and radioisotope tests. Underlying many of the problems discussed is the lack of a technical basis for specifications on maximum allowable leak rates and contaminant levels; no data is available to relate leak rate to component life. Of concern is the proliferation of test conditions which has complicated testing and test intercomparison efforts, and has resulted, unwittingly, in testing devices to significantly different actual leak rate criteria. Water vapor, sealed-in and that which penetrates the package, is a contaminant of major concern, and the difficulties of making sufficiently accurate measurements of water vapor were detailed. The control required in the materials and assembly process to avoid hermeticity failure and false leak indications in ceramic, dual in-line packages were discussed. Finally, the importance of performing some hermeticity tests at elevated temperatures was cited.

SP400-10. **Semiconductor Measurement Technology: Spreading Resistance Symposium.** Proceedings of a Symposium held at the National Bureau of Standards, Gaithersburg, Md., June 13-14, 1974, J. R. Ehrestein, Ed., Nat. Bur. Stand. (U.S.), Spec. Publ. 400-10,293 pages (Dec. 1974) SD Catalog No. C13.10:400-10, $3.55.

Key words: dopant concentration; dopant profiles; metal-semiconductor contacts; resistivity; semiconductor surface preparation; silicon; spreading resistance.

This Proceedings contains the information presented at the Spreading Resistance Symposium held at the National Bureau of Standards on June 13-14, 1974.

This Symposium covered the state of the art of the theory, practice and applications of the electrical spreading resistance measurement technique as applied to characterization of dopant density in semiconductor starting materials and semiconductor device structures. In addition to the presented papers, the transcripts of the discussion sessions which were held directly after the Theory, Practice and Applications sessions are also included. These transcripts, which were reviewed by the respective respondents for clarity, are essentially as presented at the Symposium.

SP405. **Benchmarking and workload definition: A selected bibliography with abstracts,** J. L. Walkowicz, Nat. Bur. Stand. (U.S.), Spec. Publ. 405, 46 pages (Nov. 1974) SD Catalog No. C13.10:405, $1.05.

Key words: benchmarking; bibliography; computer performance measurement; computer procurement; workload definition.

These 85 citations to the literature of benchmarking and workload definition were selected from a longer list of documents, encompassing a somewhat broader scope, that was submitted to Federal Information Processing Standards (FIPS) Task Group 13 in response to a request made to attendees of the Task Group's Planning Session held on July 12, 1973, at the National Bureau of Standards. One of the topics discussed at the Planning Session was the collection of a selected bibliography on workload definition and benchmarking. The bibliographic effort was to be directed not so much toward exhaustiveness as toward the development of a bibliography that the attendees had found useful and would, therefore, recommend to other workers in the field. Of the approximately 250 citations submitted to the Task Group, these 85 were selected on the basis of two criteria: (1) the item dealt primarily with benchmarking or workload definition; and (2) hard copy was available at the Institute for Computer Sciences and Technology. The citations are arranged alphabetically by last names of the first authors. Each citation has an abstract, a classification category assignment, and a list of keywords. The category assignments are made from a classification scheme that was developed for the collection and that is used here as a Category Index to the Bibliography. A Keyword Index is also provided.

SP409. **Marine pollution monitoring (petroleum).** Proceedings of a Symposium and Workshop Held at the National Bureau of Standards, Gaithersburg, Md., May 13-17, 1974, R. C. Junghans, Conference Coordinator, Nat. Bur. Stand. (U.S.), Spec. Publ. 409, 293 pages (Dec. 1974) SD Catalog No. C13.10:409, $3.90.

Key words: analytical methods; data reporting procedures; Intergovernmental Oceanographic Commission (IOC); marine pollution (petroleum) monitoring; Maritime Administration (MarAd); National Bureau of Standards (NBS); National Oceanic and Atmospheric Administration (NOAA); oil slicks and tar balls; petroleum hydrocarbon measurement; sampling methods; World Meterological Organization (WMO).

These proceedings contain the invited plenary lectures representing pertinent scientific, environmental, and regulatory aspects of petroleum hydrocarbon measurements, the summaries of the contributed papers, dealing with specific scientific developments and recommendations, and the recommendations of the topical discussion groups. Also included is a report of an international workshop which provides specific recommendations for the initiation of a coordinated Pilot Project for marine pollution (petroleum) monitoring.

SP411. **Fire safety research.** Proceedings of a Symposium held at the National Bureau of Standards, Gaithersburg, Md., August 22, 1973, M. J. Butler and J. A. Slater, Eds., Nat. Bur. Stand. (U.S.), Spec. Publ. 411, 251 pages (Nov. 1974), $3.10.

Key words: children; flammable fabrics; sleepwear; standards development; statistics.

The general methodology used in the development of a mandatory flammability Standard is presented. An illustrative summary is given of the hazard analysis of the accident data and the subsequent test development and laboratory investigations conducted in the development of the children's sleepwear flammability standards (DOC FF-3-71 and DOC PFF 5-73). Some of the problems encountered in the development of a mandatory standard and the resolution of those problems are discussed.

SP412. **Aerosol measurements.** The Proceedings of a Seminar on Aerosol Measurements, May 7, 1974, W. A. Cassatt and R. S. Maddock, Eds., Nat. Bur. Stand. (U.S.), Spec. Publ. 412, 193 pages (Oct. 1974) SD Catalog No. C13.10:412, $2.65.

Key words: aerosol instrument performance; aerosol measuring instruments; beta-ray absorption; Doppler shift; electromobility; laser light scattering; optical imaging; piezoelectric effect.

Papers followed by discussions were given in a closed seminar and workshop sponsored by the National Bureau of Standards and the Food and Drug Administration to define the state of development of aerosol measuring instruments. The instruments discussed were based upon a variety of operating principles including laser light scattering, optical imaging, Doppler shift, electromobility, piezoelectric effect, and beta-ray absorption. Two review papers were given which described other phenomena upon which aerosol measurements are based. The general summary includes a table which lists the specifications of the instruments discussed to illustrate the range of capabilities available in this field. Discussion among seminar attendees revealed that many questions remain to be answered before the more difficult aerosol measurements problems can be solved. For example, in the analysis of very dense aerosols questions arise concerning coincidence losses or agglomeration effects that may result from collisions between particles as they are drawn into the measuring volume. Volatilization or condensation effects may alter the size distribution if the measurements are made late in time. Finally, variations in particle shape or index of refraction can alter the instrument response and cause difficulties in interpretation.

SP414. **Laser induced damage in optical materials: 1974.** Proceedings of a Symposium Sponsored by Office of Naval Research, The American Society for Testing and Materials, and by the National Bureau of Standards, May 22-23, 1974, NBS, Boulder, Colo., 80302, A. J. Glass and A. H. Guenther, Eds., Nat. Bur. Stand. (U.S.), Spec. Publ. 414, 256 pages (Dec. 1974) SD Catalog No. C13.10:414, $3.15.

Key words: IR windows and mirrors; laser damage; laser materials; self-focusing; thin films.

The Sixth ASTM-ONR-NBS Symposium on Laser Induced Damage in Optical Materials was held at the National Bureau of Standards in Boulder, Colo., on May 22-23, of this year. These Symposia are held as part of the activities in Subcommittee II on Lasers and Laser Materials, of the ASTM. Subcommittee II is charged with the responsibilities of formulating standards and test procedures for laser materials, components, and devices. The Chairman of Subcommittee II is Haynes Lee, of Owens-Illinois, Inc. Co-chairmen for the Damage Symposia are Dr. Arthur Guenther, Chief Scientist of the Air Force Weapons Laboratory, and Dr. Alexander J. Glass, Head, Theoretical Studies, Y Division, Lawrence Livermore Laboratory.

Over 150 attendees at the Symposium heard 31 papers on topics relating to laser induced damage in crystalline and non-linear optical materials, at dielectric surfaces, and in thin film coatings as well as discussions of damage problems in the infrared region due both to cw and pulsed irradiation. In addition, several reports on the theoretical

analysis of laser-materials interaction relative to the damage process were given, along with tabulations of fundamental materials properties of importance in evaluation of optical material response to high power laser radiation. Attention was given to high power laser system design considerations which relate to improved system performance and reliability when various damage mechanisms are operable in such systems.

Because of the growing importance and acceptance of machined components in high power laser systems, a workshop on the machining of optics was held, under the coordination of Captain T. T. Saito of the Air Force Weapons Laboratory. Nine papers on various facets of the topic were presented dealing with machining procedures, surface characterization of machined elements, coating of machined components, and the polishing and damage resistance of polished, coated, and bare metal reflectors. Abstracts on these papers are included in the Symposium Proceedings proper.

The proceedings of these Symposia represent the major sources of information in the field of laser induced damage in optical materials. The Symposia themselves, along with the periodic meetings of Subcommittee II, provide a unique forum for the exchange of information regarding laser materials specifications among the manufacturers and users of laser devices, components, and systems. The Symposia also serve as a mechanism of information gathering to enable the Subcommittee to write informed and realistic specifications.

NSRDS-NBS49. **Transition metal oxides. Crystal chemistry, phase transition and related aspects,** C. N. R. Rao and G. V. Subba Rao, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 49, 138 pages (June 1974) SD Catalog No. C13.48:49, $1.70.

Key words: critical data, transition metal oxides; crystal structure transformations; electronic properties; magnetic properties; phase equilibria; phase transitions.

A survey is made of the data describing the thermodynamics of phase equilibria, crystal chemistry and phase transformations of binary oxides of 3*d*, 4*d*, and 5*d* transition metals. Changes in electrical, magnetic, and other properties which accompany phase transitions are discussed. Nearly complete coverage of the literature is provided up to 1973.

BSS55. **Preliminary performance criteria for bituminous membrane roofing,** R. G. Mathey and W. C. Cullen, Nat. Bur. Stand. (U.S.), Bldg. Sci. Ser. 55, 16 pages (Nov. 1974) SD Catalog No. C13.29/2:55, 65 cents.

Key words: bituminous roof membranes; performance attributes; performance criteria; physical and engineering properties; test methods.

This report is the first in a series of publications on performance criteria for built-up roof membranes. The development of a performance approach to bituminous built-up roof membranes is described and preliminary performance criteria are recommended. A number of test methods have been developed in order to obtain data to evaluate roofing membranes against the recommended criteria. Twenty attributes that effect the performance of roof membranes under service conditions are identified and laboratory tests are described for measuring the engineering properties of the membrane that pertain to many of these attributes. A level of performance is recommended for nine of the identified performance attributes.

BSS56. **Development of improved design criteria for low-rise buildings in developing countries to better resist the effects of extreme winds,** *Proceedings of a Workshop held at the Dr. Paulino J. Garcia Memorial Hall, National Science Development Board, Manila, Philippines, Nov. 14-17, 1973,* N. J. Raufaste, Jr., and R. D. Marshall, Eds., Nat. Bur. Stand. (U.S.), Bldg. Sci. Ser. 56, 171 pages (Oct. 1974) SD Catalog No. 13.29/2:56, $2.35.

Key words: codes and standards; information transfer; low-rise buildings; pressure transducers; socio-economic; structural design; technology implementation; wind effects; wind loads.

An International Workshop held in Manila, Philippines, on November 14-17, 1973, addressed the state-of-the-art in mitigating building damages from winds. The workshop was jointly sponsored by the United States Agency for International Development (USAID), the Philippine Advisory Committee (formed in conjunction with this research project), and the U.S. National Bureau of Standards (NBS). This report presents the proceedings derived from the workshop. The proceedings present recommendations, the workshop program, five reports, and nine technical articles. The technical articles addressed four primary topics which were used to guide subsequent workshop discussions. The topics addressed were: wind and aerodynamics, structural related technology, socio-economic and architectural considerations, and codes and standards.

The results of the workshop will serve a twofold purpose. The first suggests improved building practices for developing countries. This was accomplished through the development of recommendations designed to upgrade to a minimum acceptable level design critera for low-rise buildings. The second involves integrating appropriate workshop information into the overall three-year AID sponsored research project to develop improved design criteria for low-rise buildings in developing countries to better resist the effects of extreme winds.

BSS58. **State-of-the-art of structural test methods for walls, floors, roofs and complete buildings,** C. W. C. Yancey and L. E. Cattaneo, Nat. Bur. Stand. (U.S.), Bldg. Sci. Ser. 58, 136 pages (Nov. 1974) SD Catalog No. C13.29/2:58, $2.00.

Key words: building construction; complete buildings; floors; roofs; standardization; test methods; walls.

As part of a comprehensive research program concerned with the structural testing of building components, conducted for the U.S. Department of Housing and Urban Development (HUD), a search for information was conducted. This search was undertaken in order to document existing information pertaining to structural testing of wall, floor and roof assemblies. Various information sources were consulted to trace the evolution of structural testing of building construction from the 1930's to the present time. This task was a prerequisite to defining the state-of-the-art and to identifying the test areas requiring fundamental research.

Based on information obtained from a review of the literature and from liaison with committees concerned with the development and revision of voluntary standards, it was found that there is a dearth of research information contributing directly to the development of test methods. Most of the research conducted on building components has been carried out either to observe the behavior of a sample of a particular type of construction or to evaluate the performance of a specimen against some performance requirements. However, helpful interferences can be made on the basis of some of the documentation, especially that contained in reports of full-scale tests on housing.

As a result of comparing the test methods used by the National Bureau of Standards in HUD project Operation BREAKTHROUGH with American Society for Testing and Materials (ASTM) Standard methods, several recommendations have been made by the authors for improving present structural test practice.

An up-to-date status report of voluntary test standards activities (in the U.S.) was prepared through verbal and written communication with members of the technical subcommittees of ASTM Committee E-6 on Performance of Building Construction.

BSS59. **The adherence of porcelain enamel to aluminum,** M. A. Baker, Nat. Bur. Stand. (U.S.), Bldg. Sci. Ser. 59, 39 pages (Nov. 1974) SD Catalog No. C13.29/2:59, $1.30.

Key words: adherence; aluminum; electron microprobe; electron microscope; porcelain enamel; spalling; x-ray diffraction.

Electron microscopy, electron microprobe, and x-ray diffraction techniques were used to determine the mechanisms of adherence of porcelain enamel to aluminum. Adherence appears to depend upon diffusion of aluminum into the enamel and further, the diffusion zone should be relatively free of reaction products for the enamel-metal system to retain good adherence after exposure to chemical solutions or to weathering. Round-robin testing of 6063 aluminum extrusions indicated that this alloy could be enameled if care were exercised in the selection of the enamel and the pretreatment.

BSS64. **Retrofitting existing housing for energy conservation: An economic analysis,** S. R. Petersen, Nat. Bur. Stand. (U.S.), Bldg. Sci. Ser. 64, 76 pages (Dec. 1974) SD Catalog No. C13.29:2/64, $1.35.

Key words: benefit-cost analysis; building economics; building envelope; economic analysis; economic efficiency; energy conservation; engineering economics; insulation; life-cycle costs; marginal analysis; thermal efficiency.

This study examines the economic aspects of energy conservation techniques suitable for retrofitting into existing housing, including insulation, storm windows and doors, and weather stripping. The objective of this study is to determine that combination of techniques which will maximize net dollar savings in life-cycle operating costs for heating and cooling operations in existing homes, subject to specific climate conditions, fuel costs, and retrofitting costs. Using microeconomic marginal analysis we find that such a combination must be economically balanced (i.e., the ratio of savings to cost must be equal at the margin for each technique) and that each technique should be utilized up to the point where the present value of the life-cycle savings generated by the last increment will just cover the costs of that last increment. Thermal engineering data is combined with the economic analysis in a computer-assisted model which estimates such optimal combinations for a wide range of climatic conditions and fuel costs. These combinations include levels of application higher than what has been previously recognized as "economical."

FIPS PUB 12-2. **Federal information processing standards index,** H. E. McEwen, Standards Coordinator, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS PUB) 12-2, 195 pages (1974) SD Catalog No. C13.52:12-2, $2.80.

Key words: American National Standards; computers; data elements and codes; data processing systems; Federal Information Processing Standards; management information systems; International Organization for Standardization; standards; U.S. Government.

This publication provides material concerning standardization activities in the area of information processing at the Federal, National, and International levels. Also included are related policy and procedural guideline documents. A list of Federal Government participants involved in the development of Federal Information Processing Standards is provided. This FIPS PUB is revised and updated annually. Supersedes NBS FIPS PUB 12-1.

FIPS PUB 32. **Optical character recognition character sets,** P. Mantek, Standards Coordinator, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS PUB) 32, 78 pages (1974) SD Catalog No. C13.52:32, $1.40.

Key words: alternate character; centerline drawings; character positioning; character sets; character shape; character sizes; font; lower case character; Optical Character Recognition; upper case character.

This standard provides the description, scope, and identification for standard sets of graphic shapes to be used in the application of Optical Character Recognition (OCR) systems. Two font styles, known as Style A and B, are described. Style A comprises a font of 92 characters which is designed to provide a maximum of machine efficiency in reading under a wide variety of applications. Style B comprises a font of 96 characters, which stresses esthetic appearance, but which may be applied under a substantial range of applications. Three sizes of characters designated as Size I, III and IV are presented. The basic requirements related to character positioning are also specified. Individual character drawings for both styles of character sets are included.

TN655. **Cryogenic refrigerators—an updated survey,** T. R. Strobridge, Nat. Bur. Stand. (U.S.), Tech. Note 655, 12 pages (June 1974) SD Catalog No. C13.46:655, 30 cents.

Key words: cost; cryogenic refrigerators; efficiency; volume; weight.

In 1969, we gave efficiency, weight, volume, and cost data for 95 cryogenic refrigerators and liquefiers excluding air separation plants. Recently, the survey was repeated. The original data and those for 49 additional refrigerators and liquefiers are presented spanning refrigeration capacities from 0.2 to 10^6 W and temperatures from 1.85 to 90 K. Generally, there is no change in the trends exhibited by the older data except that the high temperature, low capacity new units seem to be larger, heavier, and slightly less efficient than in prior years. Presumably, these effects are due to efforts to increase useful life and reliability. Costs remain the same as predicted before even though no dollar value adjustments were made.

TN661. **Advances in the measurement of rf power and attenuation using SQUIDS,** R. A. Kamper, M. B. Simmonds, R. T. Adair, and C. A. Hoer, Nat. Bur. Stand. (U.S.), Tech. Note 661, 27 pages (Sept. 1974) SD Catalog No. C13.46:661, 80 cents.

Key words: Josephson effect; quantum interference; rf attenuation; rf measurement; rf power; superconductivity.

This report covers the progress made in the application of Superconducting QUantum Interference Devices (SQUIDs) to the measurement of rf power and attenuation during the year from July 1973 to June 1974. The earlier work on this project was reported in NBS Technical Note 643, which contains a detailed introduction to the principles involved. We will assume the reader to be familiar with the material we presented there, since we do not repeat it in this report. In order to make the connection as smooth as possible, we have retained our earlier chapter titles as far as possible.

During the year we have developed stable SQUIDs with preset junctions which survive thermal cycling and mechanical shock. Further work is required to arrive at a version suitable for precise rf measurements. We have assembled a "breadboard" system capable of measuring rf power at levels down to 10^{-15}W in the range of frequency from 100 MHz to 1 GHz. We have extended the dynamic range of our system to measure rf attenuation to 60 dB, and developed the hardware to partially automate its operation and to accommodate step attenuators. We have tested a portable version of this system, and are in process of designing an improved version based on what we learned from the first one.

TN835. **Tabulation of published data on electron devices of the U.S.S.R. through December 1973,** C. P. Marsden, Nat. Bur. Stand. (U.S.), Tech. Note 835, 130 pages (Nov. 1974) SD Catalog No. C13.46:835, $1.95.

Key words: electron devices; electron tubes; semiconductors; U.S.S.R.

This tabulation includes data on U.S.S.R. electron devices as collected from publications, mostly handbooks, published by the various ministries and institutes of the U.S.S.R. Information is given on all active devices ranging from receiving to microwave devices, semiconductor devices, and miscellaneous devices such as photographic flash tubes and thermistors. Supersedes NBS TN715.

TN847. **Dataplot 70: Fortran-callable plotting routines,** C. V. Young and P. G. Stein, Nat. Bur. Stand. (U.S.), Tech. Note 847, 32 pages (Oct. 1974) SD Catalog No. C13.46:847, 80 cents.

Key words: digital plotter; graph; graphics; minicomputer; plotter.

A description is given of Dataplot 70, a program which enables plotting 1) lines between pairs of X-Y coordinates and 2) a string of ASCII characters at a given X-Y coordinate on the electrostatic printer/plotter. Detailed instructions are provided enabling the user to 1) convert data to plotter format, 2) draw axis, 3) label axis, 4) scale data, 5) handle arrays, 6) produce symbols at end points, and 7) offset the origin. Hardware and software requirements as well as loading and operating instructions are given.

A sample FORTRAN calling program is included and each instruction is explained in detail. The output of the calling program is shown. Error messages produced by Dataplot 70 are explained.

TN851. **Computer system capacity fundamentals,** D. J. Kuck, Nat. Bur. Stand. (U.S.), Tech. Note 851, 25 pages (Oct. 1974) SD Catalog No. C13.46:851, 80 cents.

Key words: capacity; computer; evaluation; measurement; performance.

A framework for the study of computer capacity is given by means of a definition of capacity in terms of speeds of various parts of a computer as well as memory size. The calculation of theoretical capacity is given for several combinations of processor, memory, and I/O bandwidth for both overlapped and nonoverlapped machines. The tradeoff between primary memory size and I/O bandwidth is discussed in terms of the new definition.

TN852. **A study of wind pressures on a single-family dwelling in model and full scale,** R. D. Marshall, Nat. Bur. Stand. (U.S.), Tech. Note 852, 40 pages (Oct. 1974) SD Catalog No. C13.46:852, 85 cents.

Key words: aerodynamics; boundary layers; buildings; codes and standards; wind loads; wind tunnels.

Wind pressures measured on a single-family dwelling are compared with results obtained from a 1:80 scale model placed in a turbulent boundary layer. It is shown that the fluctuating components of surface pressures far exceed the mean or steady pressures and are well correlated over sizeable roof areas. The consistently low fluctuating pressure coefficients obtained from the wind tunnel model are attributed to improper simulation of the lower portion of the atmospheric boundary layer. Comparisons between actual loads and specified design loads suggest that certain current provisions are marginal for tributary areas and excessive for localized areas such as ridges, eaves and corners. A procedure for expressing loads on both localized and extended roof areas in terms of mean pressure coefficients and a peak factor is described.

NBSIR 73-210. **LEAA police equipment survey of 1972. Volume I: The need for standards—priorities for police equipment,** R. Ku, E. Bunten, and P. Klaus, 212 pages (July 1973). Order from NTIS as COM 74-11767, $7.25.

Key words: police; police equipment; standards.

The report describes the methodology of and summarizes a portion of the data from the LEAA Police Equipment Survey of 1972. One of a series of seven reports resulting from this nationwide mail survey of a stratified random sample of 1386 police departments, the present report summarizes the answers of 1100 police departments concerning the need for performance standards for items of law enforcement used in their departments. Each sample department was asked to rank one list of equipment categories and nine lists of equipment items within those categories in terms of the need for standards for those equipment within their own departments. The data are presented by all responding departments, by all city departments, by seven department types, and by ten LEAA geographical regions. Data describing the characteristics of the responding departments are also presented.

NBSIR 73-213. **LEAA police equipment survey of 1972. Volume IV: Alarms, security equipment, surveillance equipment,** J. L. Eldreth, E. D. Bunten, and P. A. Klaus, 147 pages (July 1971-Oct 1973). Order from NTIS as COM 74-11771, $5.75.

Key words: alarm systems; cameras; police; police equipment; security equipment; surveillance equipment.

The report outlines the methodology of and summarizes a portion of the data from the LEAA Police Equipment Survey of 1972. One of a series of seven reports resulting from this nationwide mail survey of a stratified random sample of police departments, the present report summarizes the answers of 447 police departments concerning their use of alarm systems, cameras, security equipment, and surveillance equipment: purchasing practices, typical patterns of use, and needs for standards for such equipment. The data are presented by all responding departments and by seven department types.

NBSIR 73-233. **Non-metallic antenna-support materials,** D. E. Marlowe, N. Halsey, R. A. Mitchell, and L. Mordfin, 53 pages (Apr. 1973). Order from NTIS as COM 74-11770, $4.25.

Key words: composite materials; end fittings for FRP rod; environmental resistance of GRP rod; fiber-reinforced-plastic rod; glass-reinforced-plastic rod; guys, antenna; mechanical properties of GRP rod; pultrusion; reinforced plastic rod; stress rupture of GRP rod.

A program was initiated to develop a non-conductive FRP rod material for use as guy lines and catenaries in large antenna systems. It is intended that the longterm structural properties of the new material, under adverse weathering conditions, be superior to those exhibited by the GRP rod and rope materials which are available at the present time. Two new end fittings for FRP rod were developed which out-perform commercially available fittings. These two fittings, which enable the tensile strengths of the rod materials to be accurately determined, include a shear-type fitting and a compression-type fitting. Deficiencies in the physical characteristics of existing GRP rod materials were identified, and modifications to the manufacturing processes were proposed to overcome these deficiencies. A subcontract was let for the manufacture of experimental GRP rods using the modified processes. A bank of six high-capacity creep testing machines was designed and is being assembled. These machines, which will accomodate long specimen lengths, are equipped with environmental chambers to permit stress-rupture testing under elevated temperature and saturated humidity conditions.

NBSIR 73-335. **Calibration of radio receivers to measure broadband interference,** E. B. Larsen, 75 pages (Sept. 1973). Order from NTIS as COM 74-11051, $4.00.

Key words: broadband interference; field strength meter; impulse standards; receiver bandwidth calibration; spectral intensity.

This report covers one phase of a project to improve the accuracy for calibrating field-strength to measure broadband signals, especially impulse interference. The amplitude of a narrowband signal is commonly expressed in μV, and a broadband signal is expressed in μV/MHz bandwidth. A future report (2nd phase) will deal with standards and techniques for producing a known impulse field to calibrate an antenna-receiver system in $\mu V/(m \cdot MHz)$. The technique used for initial calibration of a receiver as an RF voltmeter is new, employing a special L-pad with 48 Ω input resistor and 2 Ω output resistor across the receiver. The input power across 50 Ω is leveled, producing a low-impedance, constant-voltage source at the receiver input terminal.

Broadband interference is generally divided into two types: (a) random noise is best characterized by its power spectral density, and (b) impulse interference (uniform periodic pulses) is best quantified by its impulse strength. Several possible approaches were evaluated for defining and measuring various bandwidths of a receiver. The response of a receiver to impulses, as measured with a peak-reading detector, is proportional to the product of receiver impulse bandwidth and signal impulse strength. Of the two types of impulse sources evaluated here (pulsed DC and pulsed RF), the latter appears to be the most accurate and repeatable. We were able to produce a clean RF pulse, choosing an effective duration of 0.1 μs in our experiments, which covered a frequency range of 100 to 1000 MHz. The worst-case uncertainty of this standard source for calibrating receiver impulse bandwidth is $\pm$ 0.7 dB.

NBSIR 73-342. **The thermophysical properties of methane, from 90 to 500 K at pressures to 700 bar,** R. D. Goodwin, 279 pages (Oct. 1973). Order from NTIS as COM 73-11978/IAS, $6.50.

Key words: densities; enthalpies; entropies; equation of state; internal energies; isobars; isochores; isotherms; Joule-Thomson inversion; latent heats of vaporization; melting line; orthobaric densities; PVT data; specific heats; speeds of sound; vapor pressures.

Thermophysical properties of methane are tabulated at uniform temperatures from 90.68 to 500 K along isobars to 700 bar. A novel equation of state is employed for the first time, having origin on the vapor-liquid coexistence boundary. Computations are based almost entirely on ideal gas specific heats and experimental P-ρ-T data via the equation of state, without weighting to data for derived properties. Good agreement with such data confirms validity of the equation and method. New P-ρ-T data are reported at 0.3 to 1.7 times the critical density.

NBSIR 73-349. **Characterization of a superconducting coil composite,** C. W. Fowlkes, P. E. Angerhofer, R. N. Newton, and A. F. Clark, 51 pages (Dec. 1973). Order from NTIS as COM 74-10241, $5.75.

Key words: composite; low temperature; Poisson's ratio; superconductor; thermal expansion; Young's modulus.

The superconducting coil composite material being utilized by the Annapolis Laboratory of the Naval Ship Research and Development Center is characterized by its mechanical and thermal properties. The Young's moduli, Poisson's ratios, and thermal contractions are measured from room temperature to 4K and reported in this interim report. A micromechanical analysis based upon volume fractions of constituents is used to predict room-temperature properties, and a comparison is made to the measured values.

NBSIR 73-406. **Reference materials for the determination of trace elements in biological fluids,** P. D. LaFleur, 22 pages (Dec. 1973). Order from NTIS as COM 74-11352, $4.25.

Key words: arsenic; biological fluids; chromium; copper; fluorine; lead; nickel; reference materials; selenium; trace elements; urine.

The preparation of a number of reference materials for the analysis of trace elements in biological standards is described. The standards produced include mercury in urine at three concentration levels, five elements [Se, Cu, As, Ni, Cr] in freeze-dried urine at two levels, fluorine in freeze-dried urine at two levels, and lead in whole blood at two concentration levels. These reference materials have been analyzed for the element(s) of interest by one or more analytical techniques, and are supplied with known concentration levels.

NBSIR 73-418. **Test methods for determining coaxial cable response to bending strain, bulk compression (hydrostatic pressure), axial strain, and torsional strain,** J. F. Mayo-Wells, S. Edelman, and J. Jacobs, 119 pages (July 1973). Order from NTIS as COM 74-11783, $5.25.

Key words: cable; coaxial; mechanical; response; strain.

Test methods have been developed for measuring the response of specimen one-meter lengths of coaxial cables, considered as sensing elements, to four separate types of strain: bending strain, bulk compression, axial tension, and torsional strain. Measurements were made on commercially available coaxial cables made in the laboratory from insulated wire and wire braid. Cable dielectric materials investigated include tetrafluoroethylene (TFE), fluorinated ethylene propylene (FEP), cellular FEP, polyethylene, cellular polyethylene, and polyvinyl chloride. Data from the measurements are included in appendixes.

NBSIR 74-357. **A modified Benedict-Webb-Rubin equation of state for parahydrogen,** R. D. McCarty, 74 pages (Feb. 1974). Order from NTIS as COM 74-10551, $6.75.

Key words: critical point; equation of state; hydrogen; index of refraction; PVT; saturation properties; scaling laws.

A 32 term modified Benedict-Webb-Rubin equation of state has been applied to data for parahydrogen. The adjustable parameters in the equation of state were determined using data from the triple point to 2500 K, with pressures to 680 atmospheres. Extensive modifications have been made to the previously accepted PVT surface for the saturated liquid and vapor phases in the near critical region. These modifications have been made on the basis of subsequent refractive index data and the application of scaling law equations. Comparisons between experimental and calculated data are given.

NBSIR 74-359. **Semi-annual report on materials research in support of superconducting machinery,** L. L. Sparks, F. R. Fickett, J. G. Hust, P. J. Giarratano, H. M. Ledbetter, E. R. Naimon, W. F. Weston, M. B. Kasen, R. L. Tobler, R. P. Mikesell, R. L. Durcholz, C. W. Fowlkes, and R. P. Reed, 313 pages (Mar. 1974). Order from NTIS as AD 780596, $13.00.

Key words: composites; fracture; liquid helium; mechanical properties; structural materials; superconducting machinery; thermal conductivity.

Results of six months research are reported to the sponsor, the Advanced Research Projects Agency of the Department of Defense.

Subjects include magneto-thermal conductivity, thermal conductivity, composites, elastic properties, fracture toughness, fatigue, and tensile. All measurements include the temperature range 4 to 300 K. Materials examined are those either presently being used in superconducting machinery or considered for use in future prototypes. Material classes include stainless steels, inconels, titanium alloys, and composites.

Special results include: the thermal conductivity in a magnetic field is considerably lower than would be predicted; a comprehensive review of glass-reinforced composite behavior at low temperatures is included; the elastic moduli of 12 engineering alloys from 4 to 300 K are reported; and fracture toughness and fatigue crack growth rate data on AISI 304, AISI 316, A286, Ti-5Al-4V and Ti-6Al-2.5 Sn at 4, 76 and 300 K have been measured.

NBSIR 74-361. **Electromagnetic interference measurements at ASA, Fort Huachuca, Arizona,** H. E. Taggart and J. W. Adams, 72 pages (Dec. 1973). Order from NTIS as COM 74-11222, $3.00.

Key words: APD; field strength; interference; power lines.

This report describes the work performed for the U.S. Army Security Agency Test and Evaluation Center (USASATEC), Fort Huachuca, Ariz. during the period from April 1973 to November 1973. The purpose of the project was to measure, analyze, and evaluate the electromagnetic environment at selected sites and to recommend methods of reducing the present levels of electromagnetic interference (EMI). The chief sources of EMI were the power lines in the area and sferics from thunderstorms. Both broadband EMI measurements and amplitude probability distribution measurements were made. Both electric and magnetic fields were measured. The frequency range covered was 15 kHz to 10 GHz. Measurements were made at three locations: 1) at Fort Huachuca USASATEC; 2) Willcox Dry Lake; and 3) Boulder, Colo. The report contains the test results, conclusions, and recommendations.

NBSIR 74-363. **Heat transfer in pulsed superconducting magnets,** V. Arp, P. J. Giarratano, R. C. Hess, and M. C. Jones, 137 pages (Jan. 1974). Order from NTIS as COM 74-11053, $10.00.

Key words: forced convection heat transfer; pulsed power systems; pulsed superconducting magnets; superconductor losses; supercritical helium; transient heat transfer.

The first section of this report summarizes design problems for the development of advanced superconducting pulse magnets, leading to recommendations for future work, primarily in (1) evaluation of eddy-current, hysteresis, and frictional losses, and (2) transient heat transfer between the superconductor and the helium. Two subsequent sections report measurements of forced convection heat transfer respectively to subcooled liquid helium and to supercritical helium just above the critical pressure.

NBSIR 74-364. **Detection of human intruders by low frequency sonic interferometric techniques,** R. E. Stoltenberg, 94 pages (May 1974). Order from NTIS as COM 74-11208, $4.00.

Key words: human detector; interferometric technique; low frequency acoustics.

This report examines the theory and evaluates the results of over 200 tests of the use of low frequency sonic interference techniques for the detection of a human intruder in a confined area. The conclusions are that this technique is potentially a significant improvement over conventional methods with regard to area coverage and minimum velocity detection.

This work examined the intruder signature and background noise with respect to sonification frequency, source levels, intruder size, intruder velocity, source types, area coverage (to 692 sq. meters), and geometric position of the source and receiver in four radically different areas.

Interference effects of the intruder signature and noise were analyzed with respect to bandwidth, spectral content, and magnitude by both computer drawn spectral displays, and specific frequency correlators.

NBSIR 74-365. **Impulse spectral intensity—what is it?,** M. G. Arthur, 25 pages (May 1974). Order from NTIS as COM 74-11375, $4.50.

Key words: electromagnetic interference; Fourier transform; impulse spectral intensity; spectral intensity; spectrum amplitude; spectrum amplitude density.

The term, impulse spectral intensity, is often used in discussions concerning electromagnetic interference and broadband signal processing. In these discussions, the term is not used in a consistent manner, resulting in confusion, equivocation, and sometimes, errors. As a step towards improving this situation, the mathematical basis for spectral intensity is reviewed and certain of its features are clarified. Also, misuses of spectral intensity are discussed, along with its limitations and proper use.

NBSIR 74-366. **Study of cryogenic propellant systems for loading the space shuttle,** R. O. Voth, W. G. Steward, and W. J. Hall, 95 pages (Apr. 1974). Order from NTIS as COM 74-11076, $8.00.

Key words: computer modeling; cooldown; cryogenic flow; stresses; surges; transient flow; water hammer.

Computer programs have been written to model the liquid oxygen loading system for the space shuttle. The programs allow selection of input data through graphic displays which schematically depict the part of the system being modeled. The computed output is also displayed in the form of graphs and printed messages. Any one of six computation options may be selected. The first four of these pertain to thermal stresses, pressure surges, cooldown times, flow rates and pressures during cooldown. Options five and six deal with possible water hammer effects due to closing of valves, steady flow and transient response to changes in operating conditions after cooldown.

Procedures are given for operation of the graphic unit and minicomputer.

NBSIR 74-369. **Surface magnetic field noise measurements at Geneva Mine,** J. W. Adams, W. D. Bensema, and N. C. Tomoeda, 40 pages (June 1974). Order from NTIS as COM 74-11688, $3.00.

Key words: earth-ionosphere waveguide; electromagnetic noise; EMI measurement technique; sferic interference.

Measurements of surface magnetic field noise were made at various locations over the Geneva Coal Mine near Price, Utah, on June 12, 1973. The locations selected were on the surface over emergency locator beacons underground at depths between 350 meters (1150 ft.) and 488 meters (1600 ft.). The surface terrain where these measurements were made was mountainous, and access was difficult. There were no power lines within several miles, and the weather was clear; therefore, the magnetic noise levels were about as low as will normally occur.

Results of measurements of distant sferics indicate rather sharp cutoff frequencies below which broadband, impulsive noise is attenuated. The mechanism of propagation for this noise above the daytime cutoff frequency of 3500 Hz and the nighttime cutoff frequency of 1700 Hz is deduced to be a waveguide formed by the D or E layers of ionosphere as an upper plane and the earth as a lower plane.

The measurement systems used are similar to those used earlier. The technique is to record broadband, analog signals, digitize the data, and use a fast-Fourier transform to obtain spectral plots. This technique is novel in that it can measure simultaneously all magnetic field energy within a limited portion of the spectrum for a limited time, and, after processing, reproduce the events occurring in that time interval in great detail.

NBSIR 74-375. **Refrigeration for an 8 K to 14 K superconducting transmission line,** D. E. Daney, 60 pages (Oct. 1974). Order from NTIS as COM 74-11657, $4.25.

Key words: Brayton cycle; refrigeration; superconducting transmission lines; superconductors.

The performance of three supercritical refrigeration cycles for cooling superconducting transmission lines has been investigated for the temperature range of 8 K to 14 K. This temperature range is applicable to the Stanford superconducting (Nb_3Sn) line. These cycles, which were selected as being the most practical, are the Brayton cycle with the expander before the load, the Brayton cycle with the expander after the load, and the Brayton cycle with a separate supercritical helium loop and circulating pump.

The results are presented as curves of Wc/Q (ratio of the work of compression to the refrigeration load) vs the transmission line exit pressure for various transmission line pressure and temperature drops. Contrary to popular belief, all three cycles are competitive. Maximum efficiencies (percent of Carnot) are about 25 percent.

Estimated capital and operating costs are presented as a function of transmission line temperature for several values of thermal load per length of line.

NBSIR 74-377. **Picosecond pulse generators using microminiature mercury switches,** J. R. Andrews, 44 pages (Mar. 1974). Order from NTIS as COM 74-11449, $5.25.

Key words: mercury switch; picosecond; pulse generator; pulse measurement; superconductivity.

Pulse generators have been built using microminiature mercury switches. A commercial RF coaxial switch was also evaluated as a pulse generator. A superconducting delay line ($t_r = 18$ ps, $t_d = 70$ ns) and a sampling oscilloscope ($t_r = 22$ ps) were used to measure the generated pulse 10-90 percent transition time. The best result obtained was a transition time of 39 ps. Pulse amplitudes were independently adjustable up to 50 volts. The microminiature mercury switches in general were found to give very unreliable operation.

NBSIR 74-378. **Time and amplitude statistics for electromagnetic noise in mines,** M. Kanda, 59 pages. Order from NTIS as COM 74-11450, $6.00.

Key words: Allan variance analysis; amplitude probability distribution; amplitude statistics; average crossing rate; electromagnetic interference; electromagnetic noise; impulsive noise; interpulse spacing distribution; magnetic field strength; man-made noise; pulse duration distribution; time statistics.

The time and amplitude statistics necessary to adequately describe electromagnetic (EM) noise in mines are illustrated through computer software techniques. They are 1) Allan Variance Analyses (AVA), 2) Interpulse Spacing Distributions (ISD), 3) Pulse Duration Distributions (PDD), 4) Average Crossing Rates (ACR), and 5) Amplitude Probability Distributions (APD). These statistics are illustrated using data taken from a rather large store of raw analog data recorded in operational mines.

The curves generated for the illustrations characterize the noise environment in the mines from which the corresponding data were taken, and should aid in the design of reliable communication systems for such mines.

NBSIR 74-380. **Planar near-field measurements on high performance array antennas,** A. C. Newell and M. L. Crawford, 100 pages (July 1974). Order from NTIS as COM 74-11686, $5.25.

Key words: antennas; near-field measurements; phased arrays.

The results of measurements which apply the planar near-field measurement technique to phased array antennas are described. Fast and efficient tests are used to determine the required scan area and data point spacing. The use of these tests can reduce the amount of data required for some antennas without significantly increasing the errors in computed results.

Measurements were made at different distances from the antennas, with the probe transmitting and receiving, and for both sum and monopulse difference patterns. Comparisons between the far-field patterns computed from the near-field data and those measured on far-field ranges are presented.

NBSIR 74-382. **A study of the measurement of G/T using Cassiopeia A,** D. F. Wait, W. C. Daywitt, M. Kanda, and C. K. S. Miller, 199 pages (June 1974). Order from NTIS as AD 783433, $13.25.

Key words: accuracy; antenna; calibration; Cassiopeia A; G/T; star flux.

This report describes a study intended to estimate the best possible accuracy of measuring the ratio G/T (system gain to system noise temperature) of a satellite communication ground station using the radio star Cassiopeia A (Cas A). The concept of G/T and its measurement using a radio star is briefly discussed. Results of an extensive literature search are presented, summarizing the properties of Cas A and its vicinity described by radio astronomers in order to utilize this information to assess the accuracy of a G/T measurement. Consideration is given to atmospheric effects upon a G/T measurement using Cas A based on information available in the literature. A detailed analysis of errors for gain measurements of large ground antennas, which includes the calibration of a standard gain antenna and the transfer of the calibration of this standard to a large antenna, is provided to validate radio star flux data since this analysis is not available in the literature. The results of these efforts are utilized to show that the best possible accuracy of a G/T measurement for a ground station having a 60 ft. diameter antenna and both practical and reasonable specifications is in the neighborhood of $\pm$ 0.25 dB.

NBSIR 74-387. **Microwave measurement of coal layer thickness,** D. A. Ellerbruch and J. W. Adams, 33 pages (Sept. 1974). Order from NTIS as COM 74-11643, $3.75.

Key words: automation; coal; coal mine safety; dielectric constant; energy; microwave measurement; nondestructive testing; thickness of coal layer.

The possibility of using a microwave system to measure coal layer thickness in a mine was investigated. Measurements were made in two different mines near Pittsburgh, Pa., and near Fairview, West Virginia. Frequencies in the range 0.5 GHz-4.0 GHz were used to measure samples between 10-40 cm thick. All samples were backed with a naturally-occurring draw slate.

The results indicated a definite possibility of determining layer thickness in most cases, although anomalies may introduce enough error to give misleading results in some cases. Anomaly detection may be very useful in some cases. More experimental data and theoretical study are needed for complete verification.

Data from a model and measured data show considerable agreement. The real value of this model is to point out causes and effects, and what additional information is needed in order to obtain a measurement system that is optimum under most conditions.

The dielectric constant of coal is apparently a function of moisture content. Draw slate seems to have a significantly higher dielectric constant than coal. Also, a layer of coal having different electrical characteristics within the layer was detected with the microwave system.

This technique has great potential if fully developed. It would have significant impact in areas of energy, safety, and productivity.

NBSIR 74-388. **Electromagnetic noise in Grace Mine,** J. W. Adams, W. D. Bensema, and M. Kanda, 138 pages (June 1974). Order from NTIS as COM 74-11687, $5.75.

Key words: amplitude probability distribution; coal mine noise; digital data; electromagnetic interference; electromagnetic noise; electromagnetic pulse (chemical); emergency communications; Fast Fourier Transform; Gaussian distribution; impulsive noise; magnetic field strength; measurement instrumentation; spectral density; time-dependent spectral density.

Two different techniques were used to make measurements of the absolute value of electromagnetic noise in an operating hardrock mine, Grace Mine, located near Morgantown, Pennsylvania. Diesel-powered haulage equipment is used in this mine, and the electromagnetic noise environment it creates was measured to see how it differs from the environment created by electric-powered haulage equipment. One technique measures noise over the entire electromagnetic spectrum of interest for brief time periods. It is recorded using broadband analog magnetic tape and the noise data is later transformed to give spectral plots. The other technique records noise amplitudes at several discrete frequencies for a sufficient amount of time to provide amplitude probability distributions.

The specific measured results are given in a number of spectral plots and amplitude probability distribution plots.

NBSIR 74-389. **Electromagnetic noise in McElroy Mine,** M. Kanda, J. W. Adams, W. D. Bensema, 170 pages (June 1974). Order from NTIS as COM 74-11717, $6.25.

Key words: amplitude probability distribution; coal mine noise; digital data; electromagnetic communications; electromagnetic interference; electromagnetic noise; Fast Fourier Transform; Gaussian distribution; impulsive noise; magnetic field strength; measurement instrumentation; spectral density; time-dependent spectral density.

Two different techniques were used to make measurements of the absolute value of electromagnetic noise in and above an operating coal mine, McElroy Mine, located near Moundsville, West Virginia. 300-volt-dc and 480-volt-ac machinery was measured to see the electromagnetic environment it created. One technique measures noise over the entire electromagnetic spectrum of interest for brief time periods. It is recorded using broadband analog magnetic tape and the noise data is later transformed to give spectral plots. The other technique records noise amplitudes at several discrete frequencies for a sufficient amount of time to provide amplitude probability distributions.

NBSIR 74-390. **Electromagnetic noise in Itmann Mine,** W. D. Bensema, M. Kanda, and J. W. Adams, 113 pages (June 1974). Order from NTIS as COM 74-11718, $5.25.

Key words: amplitude probability distribution; coal mine noise, digital electromagnetic communications; electromagnetic interference; electromagnetic noise; Fast Fourier Transform; Gaussian distribution; impulsive noise; magnetic field strength; measurement instrumentation; spectral density; time-dependent spectral density.

Two different techniques were used to make measurements of the absolute value of electromagnetic noise in an operating coal mine, Itmann No. 3 Mine, located near Mullens, West Virginia. The electromagnetic environment created by 250-volt-dc and 550- and 950-volt-ac machinery in two longwall panels was measured and is reported. One technique measures noise over the entire electromagnetic spectrum of interest for brief time periods. It is recorded using broadband analog magnetic tape, and the noise data is later transformed to give spectral plots. The other technique records noise amplitudes at several discrete frequencies for a sufficient amount of time to provide amplitude probability distributions.

The specific, measured results are given in a number of spectral plots and amplitude probability distribution plots.

NBSIR 74-396. **Specification and measurement of frequency stability,** J. H. Shoaf, 44 pages (Nov. 1974). Order from NTIS as COM 74-11766, $3.75.

Key words: Allan variance; frequency stability measurements; measurement system description; phase noise; spectral density; terminology standards.

This report gives concise definitions for specifying frequency stability for measurements in the frequency domain and time domain. Standards of terminology and of measurement techniques are recommended. Measurement systems are described in adequate detail so that the apparatus may be duplicated. Proposed extension of the measurement systems through 12.4 GHz is discussed.

NBSIR 74-451. **Field comparisons of steel surveyors' tapes,** C. L. Carroll, Jr., 16 pages (Nov. 1973). Order from NTIS as COM 74-11385, $4.00.

Key words: graduation; length; scale; tape; temperature; tension.

Report describes a field procedure to compare a steel surveyor's tape to a standard tape that has been calibrated by the National Bureau of Standards. The procedure requires only a hand-held magnifier, two short scales, and two spring balances. Temperature reading device is not required since both tapes are made of steel and have the same temperature during the comparison.

NBSIR 74-456. **Evaluation of the fire performance of a dibromotetrafluoroethane–blown rigid polyurethane foam,** T. G. Lee, W. J. Parker, and M. Tryon, 17 pages (Apr. 1974). Order from NTIS as COM 74-11793, $3.25.

Key words: dibromotetrafluoroethane; fire tests; flame spread index; heat release rate; ignition temperature; rigid urethane foam; smoke.

The fire performance characteristics of a dibromotetrafluoroethane–blown rigid polyurethane foam were measured by several laboratory test methods. Measurements included: surface flammability, smoke and gases generated at elevated temperature and during combustion, ignition temperature, rate of heat release, and fire growth. The maximum concentration of the blowing agent in the specimen was approximately 13 Wt%. Specimen density was 0.046 g/cm^3. As a function of temperature, release of blowing agent from collapsed cells began at about 60 °C and became considerable at 135 °C. The material had a flame spread index (ASTM E-162) of 11 with smoke levels of 170 and 480 (maximum specific optical density) under nonflaming and flaming exposures, respectively. The measured rate of heat release was 8.8 W/cm^2, about 5 times that of a fibrous glass insulation. The measured flash ignition temperature was 530 °C for the material.

NBSIR 74-457. **Transmission of electrons through foils,** S. M. Seltzer, 84 pages (Apr. 1974). Order from NTIS as COM 74-11792, $4.75.

Key words: angular distribution; electrons; energy spectra; reflection; transmission; transport calculation.

The transmission of electrons through foils has been studied by a Monte Carlo method. Cases involving electrons with energies from 50 keV to 1 MeV normally incident on beryllium, mylar, aluminum, and titanium foils are considered. Good agreement with experimental results has been found for quantities such as the number transmission, the energy and angular distribution of the emergent electrons, and the spatial distribution of energy deposited in the foil.

A comprehensive set of results has been generated for 100, 150, 200, 300 and 400-keV electrons incident on beryllium, mylar, aluminum, and titanium foils that are commonly used as vacuum windows in conjunction with low energy electron accelerators. Quantities given are the electron number and energy transmission and reflection, the energy absorbed, and the energy and angular distribution of the transmitted electrons. It is shown that much of the results can be presented in a scaled form which reduces the explicit dependence on, and facilitates the interpolation with respect to, the incident energy.

NBSIR 74-467. **Simulated solar heat tests on M.U.S.T. air-inflatable, double-wall hospital ward shelters,** L. W. Masters, J. W. Grimes, and R. A. Crist, 64 pages (May 1974). Order from NTIS as COM 74-11754, $4.25.

Key words: adhesives; air-inflatable shelter sections; cloth webs; polyester and nylon fabrics; sewn seams; sewn seam strapping; solar heat load; test procedure.

At the request of the United States Army Natick Laboratories (USANLABS), the Center for Building Technology conducted solar heat load tests on five sections of M.U.S.T. air-inflatable, double-wall hospital ward shelters. The purpose of the tests was to evaluate the effect of solar heat load, as simulated by infrared heat lamps, on various materials and construction designs proposed for use in shelters.

NBSIR 74-473. **Natural disasters: Some empirical and economic considerations,** G. T. Sav, 72 pages (Feb. 1974). Order from NTIS as COM 74-11719, $4.25.

Key words: benefit-cost analysis; disaster mitigation; earthquakes; economics; efficient; floods; hurricanes; natural disasters; optimal; tornadoes; total cost minimization.

This study examines the extent of some of the losses resulting from natural disasters. An estimate of these losses is necessary in order to determine the potential benefits that might be realized from mitigating the negative economic impacts from natural disasters. Absolute and relative losses resulting from hurricanes, floods, earthquakes, and tornadoes are examined. This data will help individuals, communities, and the Federal government make better decisions as to how and what extent protection against disasters should be provided. The application of benefit-cost analysis for choosing the optimal level of protection against disasters is also discussed. Recommendations are made for further research in determining the economic feasibility of various techniques designed to mitigate the losses from disasters.

NBSIR 74-477. **Performance characteristics of a "bulk effect" humidity sensor,** J. W. Little, S. Hasegawa, and L. Greenspan, 33 pages (May 1974). Order from NTIS as COM 74-11784, $3.75.

Key words: "Brady Array" sensors; electric hygrometer; humidity; humidity sensor; moisture measurement; relative humidity; water vapor measurement.

A laboratory study was made of the performance of "Brady Array" humidity sensors over a range of ambient temperatures from − 40 °C to + 20 °C encompassing relative humidities from 0 to 90 percent. Information was obtained on such characteristics as sensitivity, hysteresis, temperature effect, short-term and long-term repeatability.

NBSIR 74-479. **Analysis of cost-sharing programs for pollution abatement of municipal wastewater,** H. E. Marshall and R. T. Ruegg, 145 pages (Sept. 1974). Order from NTIS as COM 74-11769, $5.75.

Key words: cost sharing; efficiency; equity; financing; nonplant treatment; sewage treatment; user fees; water pollution.

This study evaluates existing cost-sharing programs for wastewater pollution abatement as described in the Federal Water Pollution Control Act Amendments of 1972, describes alternative cost-sharing programs that provide improvements in terms of national efficiency and equity criteria as defined herein, and suggests related areas for further research. Emphasis is on how Federal cost sharing biases communities in favor of certain kinds of techniques. The approach is to describe the current cost-sharing programs for both plant and nonplant techniques; to examine cost-sharing, legal, and other institutional biases against certain techniques; to analyze efficiency and equity effects of alternative cost-sharing programs; and to describe the incentive effects of cost-sharing on nonfederal interests with respect to their choices among abatement techniques. Findings of the study are that more efficient abatement will result if the *same* percentage cost share applies to all plant and nonplant techniques of abatement; the *same* percentage also applies to all categories of cost (e.g., capital, land, operation and maintenance) for a given technique; the *same* percentage applies to large and small communities; institutional constraints on the selection of nonplant techniques are removed; and if the program provides for Federal cost sharing of every abatement technique that is technically viable.

NBSIR 74-481. **Absolute calibration of vibration standards by the three-mass reciprocity method,** J. D. Ramboz, 50 pages (Apr. 1974). Order from NTIS as COM 74-11794, $4.25.

Key words: absolute calibration; accelerometers; calibration; reciprocity calibration; vibration exciters; vibration pickups; vibration standards.

Reciprocity calibration of electrodynamic vibration exciters is reviewed. A new method is proposed. The theory for the new Three-Mass reciprocity calibration method is developed. The process requires that the electrical impedance of the exciter's drive coil be measured for three added masses separately mounted on the exciter's armature. The sensitivity of the accelerometer mounted in the armature is solved in terms of a change of electrical impedance for a change of mass, voltage ratio, electrical resistance, and frequency. A set of 38 measurements were made at 1000 Hz to experimentally verify the theory. The value of sensitivity was 2.070 pC/g ± 1.3 percent. This agreed to within about ± 0.65 percent of a transfer calibration from Bouche-Levy calibrated standards and the manufacturer's estimated value. Measurements were made to verify the theory; improvement to an uncertainty of about ± 0.2 percent is ultimately possible in the absolute calibration using this method.

NBSIR 74-486. **Reliability, life prediction and proof testing of ceramics,** S. M. Wiederhorn, 62 pages (May 1974). Order from NTIS as AD 780705, $4.25.

Key words: ceramics; crack propagation; delayed failure; fracture; proof testing; Weibull analysis.

A critical review is presented of the use of proof testing as a design method for assuring the reliability of structural components. The advantage of proof testing over the statistical approach used for design lies in the insensitivity of the proof testing method to the detailed history of handling or processing of structural components. Methods are presented for developing and using proof test diagrams to assure component lifetime after proof testing. Procedures of proof testing and precautions that must be followed during proof testing are discussed. Provided these precautions are followed, proof testing offers a general method for assuring the reliability of structural components under stress.

NBSIR 74-495. **Development of a radiant panel test for flooring materials,** L. G. Hartzell, 79 pages (May 1974). Order from NTIS as COM 74-11575, $7.00.

Key words: carpet; fire test; flammability; flooring; heat flux; ignition; radiant panel.

This paper summarizes the work of a year long program to continue the development of a radiant panel type test for flooring materials, the original concept of which was developed at the Armstrong Cork Company's Research and Development Center in Lancaster, Pennsylvania. This program at the National Bureau of Standards had as its goal, the further development of the test for possible adoption as a standard ASTM test method.

The program work was divided into five phases. During the first phase, an attempt was made to duplicate the performance of the original apparatus in a similar one at the National Bureau of Standards Laboratory. The proof of this duplication was shown in replicate testing using a wide range of flooring on both apparati.

In the second phase of the program, a new set of test conditions were found in an attempt to eliminate some of the more serious equipment and procedural problems of the test. These new conditions provided the test with the ability to rate flooring materials according to their ability to resist the surface spread flames.

Under the third and fourth phases of the program, the effects of changes in some test parameters was investigated and other test characteristics were measured. Phase V, the data analysis and report, concluded the program.

NBSIR 74-496. **Standard measurements of the resistivity of silicon by the four-probe method,** W. M. Bullis, 75 pages (Aug. 1974). Order from NTIS as COM 74-11576, $7.00.

Key words: ASTM Committee F-1; electronics; four-probe method; resistivity; semiconductors; silicon.

An improved standard procedure for measurement of circular silicon slices with four in-line point probes has been developed in cooperation with the Resistivity Task Force of ASTM Committee F-1. Detailed analysis of a series of round-robin experiments showed that the procedure can attain a precision of ± 2 percent (three standard deviations) for interlaboratory comparisons of slices with room temperature resistivity between 0.005 and 120 ohm-cm. Resistivity nonuniformity in the test slices was shown to be a significant factor in limiting the precision which could be achieved. The importance of including correction factors for temperature, finite thickness, finite diameter, and unequal probe separations was demonstrated. The results of the round-robin experiments also emphasized that the precision quoted can only be achieved if the measurements are carefully and correctly made on a well maintained, accurately calibrated test system which meets the requirements imposed by the test method. Determination of the precision to be expected from the method in nonreferee applications such as routine production and quality control will require additional study of such factors as surface conditions, probe force, current levels, etc. Nevertheless, use of the various procedures of the method, in particular the sections on probe and measuring circuit evaluations and on thermal sinking of the wafer, would be expected to yield significantly improved precision in such applications. Use of these procedures on a regular and widespread basis should be encouraged.

NBSIR 74-499. **An analysis of the aging of paper: Possible reactions and their effects on measurable properties,** W. K. Wilson and E. J. Parks, 37 pages (Apr. 26, 1974). Order from NTIS as COM 74-11378, $3.25.

Key words: accelerated aging; aging; aging of cellulose; aging of paper; cellulose; cellulose aging; natural aging; paper; paper aging; tests for paper.

Various reactions that cellulose can undergo are reviewed in relation to their bearing on the aging of paper. The principal reactions of cellulose are hydrolysis, oxidation, crosslinking, change in lateral order in the bonding area, and, during accelerated aging, thermal decomposition. The effects these various reactions might have on tests that are available for evaluating changes that occur during the aging of paper are reviewed. Some special examples of these reactions that occur during natural aging, because of special composition characteristics of the paper, are discussed. Suggestions are made concerning most sensitive tests for use in detecting changes in paper and tests, regardless of sensitivity, available for determining *what* happens during aging. Some general guidelines regarding specifications for permanent record papers are discussed.

NBSIR 74-506. **Development of a national anthropometric data base: A preliminary study report,** H. L. Steinberg, 85 pages (June 1974). Order from NTIS as COM 74-11632, $3.00.

Key words: anthropometric survey; biostereometric body-dimensions; National Data Base.

A study was made to determine the need for development of a Nationally Representative Anthropometric data base. Potential users and their needs are identified and the inability of existing anthropometric data to satisfactorily meet these needs is established. Three scenarios for developing a useful data base are considered. Two involve the use of biostereometrics while the third takes a relatively conventional approach to obtaining body dimensions. Conclusions relevant to each of these scenarios, as well as the potential advantages/disadvantages of each, are developed. Salient conclusions common to all three scenarios include: The need for a (R & D type) pilot study; the desirability of linking the actual anthropometric survey to a National Center for Health Statistics (NCHS) "Health and Nutrition Examination Survey" (HANES); and a data base development time of at least 7 years. Program costs, detailed in an appendix, ranged from $2.4M to $5.2M. Mechanisms for administering and funding this survey were considered briefly. An estimation of the optimal sampling dimensions for the proposed survey, based on clothing industry needs, is given.

NBSIR 74-509. **Strength and stability testing of high chairs,** D. J. Chwirut, 17 pages (June 1974). Order from NTIS as COM 74-11377, $3.00.

Key words: accident reports; high chairs; infants; safety standards; stability and strength; test methods.

Accident reports from hospital emergency rooms were surveyed to determine the probable causes of accidents involving high chairs. Possible test methods for determining the characteristics of the high chairs leading to the accidents were investigated, including the test methods recommended in the Juvenile Products Manufacturers Association Voluntary Safety Standard for High Chairs. These tests included tests for tray strength, chair static strength, foot rest strength, restraining strap strength, and stability. These test methods and performance characteristics are intended to supply information leading to federal safety standards.

NBSIR 74-511. **Fire research publications, 1973,** N. H. Jason, 13 pages (June 1974). Order from NTIS as COM 74-11448, $4.00.

Key words: bibliographies; building fires; construction materials; fire departments; fire tests; flame spread test; flammability tests; flammable fabrics; Operation BREAKTHROUGH; protective clothing.

A list of publications is provided representing the papers and journal articles prepared by members of the Programmatic Center for Fire Research (PCFR) and by NBS personnel under contract to PCFR and by external laboratories under contract to the PCFR during 1973.

NBSIR 74-515. **Report of conference on making service industries more productive through computers and automation,** A. K. McAdams and M. M. Henderson, 176 pages (June 1974). Order from NTIS as COM 74-11498, $5.50.

Key words: automation; computers; productivity; service industries.

The Engineering Foundation and the National Bureau of Standards, Institute for Computer Sciences and Technology, cosponsored this conference to bring together persons actively concerned with the subject to identify gaps in knowledge, needs and opportunities in the area, and to point up governmental goals and programs to respond to such needs. This report contains the principal presentations and the texts of Workshop Panel reports prepared during the conference.

NBSIR 74-519. **Photometric tests of vehicle glazing materials,** W. A. Hall, E. L. Walters, I. Nimeroff, C. A. Douglas, 33 pages (Nov. 1974). Order from NTIS as PB 238-284, $3.75.

Key words: automobile paint colors; automobile windshield color; photometric tests; spectral reflectance; spectral transmittance; transmittance variation; vehicle glazing materials.

Measurements were made on the spectral transmittance of representative vehicle glazing materials and spectral reflectance of representative automobile paints. Colorimetric data were derived from these spectral measurements.

By varying the instrumental parameters of the in-laboratory procedure described in NBS Report No. 10902 for measuring the transmittance of glazing materials, errors in transmittance were obtained and were evaluated. The standard deviation of the transmittance measurements was less than 0.01 except at incidence angles of 70° where it was about 0.02.

NBSIR 74-520. **Evaluation of structural properties of masonry in existing buildings,** S. G. Fattal and L. E. Cattaneo, 127 pages (July 1974). Order from NTIS as COM 74-11480, $3.00.

Key words: analysis; compressive strength; deflection; design; flexural strength; masonry walls; racking strength; seismic loading; shear strength; shear wall; stiffness.

The current state of knowledge on the structural behavior of masonry is synthesized to develop a methodology for the evaluation of the load capacity of masonry walls in existing buildings. A procedure is described for direct sampling and testing of specimens removed from masonry walls of buildings to determine their strength in shear, flexure and compression, and to measure their load-deformation characteristics. A documentation of strength and stiffness properties obtained from available test data is included to provide an alternate source of information on masonry of comparable construction. Sample calculations of masonry building analysis for seismic forces are given in Appendices A and B.

NBSIR 74-524. **Practicality of diversion path analysis,** W. M. Murphey, J. C. Schleter, 36 pages (July 1974). Order from NTIS as COM 74-11568, $5.00.

Key words: analysis; diversion of nuclear materials; diversion path analysis; internal control system characterization; nuclear material safeguards; safeguards.

One can define the safeguards system for nuclear material as the set of all protective actions taken to prevent or to deter attempts to divert nuclear material to unauthorized use. Maintenance of effective safeguards requires a program for routine assessment of plant safeguards systems in terms of their capabilities to satisfy safeguards aims. Plant internal control systems provide capabilities for detection of unprevented diversion and can provide assurance that diversion has not occurred. A procedure called Diversion Path Analysis (DPA) enables routine assessment of the capabilities of internal control systems in this regard and identification of safeguards problem areas in a plant. A framework for safeguards system design is also provided which will allow flexibility to accommodate individual plant circumstances while maintaining acceptable diversion detection capability. The steps of the procedure are described and the practicality of the analytical method is shown by referring to a demonstration test for a high throughput process where plant personnel were major participants. The boundary conditions for the demonstration case are given, along with some conclusions about the general procedure.

NBSIR 74-525. **Optical materials characterization,** A. Feldman, D. Horowitz, R. M. Waxler, I. Malitson, and M. J. Dodge, 20 pages (July 1974). Order from NTIS as AD 782564, $3.00.

Key words: As_2S_3; chalcogenide glass; coefficient of thermal expansion; elastic constants; infrared laser window materials; KCl; photoelasticity; polycrystalline ZnSe; refractive index; stress-optical constants; thermal coefficient of refractive index.

A program has been established for measuring refractive index, n, stress-optical constants, q_{ij}, change of index with temperature, dn/dT, thermal expansion coefficient, α, and elastic compliances, s_{ij}, of infrared laser window materials. These parameters are necessary for determining the optical distortion that occurs in windows due to heating by the absorption of high power laser radiation. n and dn/dT are measured over a spectral range 0.2 to 50 μm by the method of minimum deviation on precision spectrometers. Twyman-Green and Fizeau interferometers which operate at 0.6328 μm, 1.15 μm, and 10.6 μm, are used for measuring q_{ij}, α, dn/dT and s_{ij}. Materials currently under study are polycrystalline ZnSe, As_2S_3 glass, chalcogenide glass (Ge 33%, As 12%, Se 55%), and KCl. Results are given for n and dn/dT in KCl, and q_{ij} and s_{12} in ZnSe, As_2S_3 glass, and chalcogenide glass.

NBSIR 74-527. **Development of solid state samplers for work atmospheres,** B. Greifer, B. C. Cadoff, J. Wing, J. K. Taylor, 54 pages (June 1974). Order from NTIS as COM 74-11720, $4.25.

Key words: air analysis; air sampler; charcoal; chlorine; fluorine; gas analysis; hydrogen cyanide; hydrogen fluoride; industrial hygiene; phosphine; sodium acetate; sorber, solid; work atmosphere.

A program is described for evaluating the efficiency of solid sorbers for collecting trace quantities of hydrogen fluoride, phosphine, hydrogen cyanide, chlorine, and fluorine in work atmospheres for subsequent laboratory analysis. The gas handling and sampling instrumentation is described, and experimental results to date are presented.

Sodium acetate is a very efficient sorber for hydrogen fluoride, and its solubility in water proves to be highly advantageous for subsequent HF determination by ion selective electrode. Potassium permanganate impregnated silica gel sorbs phosphine effectively, and Ascarite has been found to sorb hydrogen cyanide, but quantitative experiments on the latter two systems are still in progress.

Work on chlorine and fluorine systems will be initiated in the near future.

NBSIR 74-529. **Project plans fiscal year 1974,** J. J. Diamond, 72 pages (July 1973). Order from NTIS as COM 74-11495, $3.75.

Key words: anthropometry; communications equipment; forensic science; Law Enforcement Standards Laboratory; LESL; performance standards; project plans; protective equipment; security equipment; standards; warning lights and sirens.

Plans are presented for nineteen projects approved and funded for FY-74. They include plans for the preparation of performance standards, user guidelines and reports on law enforcement equipment in the communications, security, protective equipment, investigative aid, emergency equipment and clothing areas.

NBSIR 74-533. **Influence of windshield tint on the temperature in automobile passenger compartments,** W. S. Hurst and M. G. Scroger, 113 pages (Sept. 1974). Order from NTIS as PB 238573, $5.25.

Key words: automobile compartment temperatures; automobile windshields; glazing materials; transmittance of vehicle glazing materials.

The effect of tinting in the glass of windshields on the air temperature in automobile passenger compartments was investigated. Measurements were performed with two nearly identical vehicles, one

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equipped with tinted windshield glass and one equipped with clear windshield glass. All other glass in both vehicles was tinted. Tests were performed statically, with the cars parked facing south, and dynamically, with the cars driven at approximately 80 km/h. In the static tests, the interior air temperatures as determined by liquid-in-glass thermometers were typically 2 to 3 °C cooler in the vehicle with the tinted windshield. In the dynamic tests, the differences in the interior air temperatures were smaller, typically about 0.5 to 1.5 °C. The interior air temperature differences determined with thermocouples varied with the thermocouple position. The differences typically ranged from a negligible amount (less than 1 °C) to about 6 °C; temperature differences as large as 16 °C were observed on the car dash.

NBSIR 74-535. **A selected and annotated bibliography of compilations of data relevant to biochemical thermodynamics,** G. T. Armstrong, G. R. Janes, and R. N. Goldberg, 81 pages (July 1974). Order from NTIS as COM 74-11659, $4.75.

Key words: bibliography; biochemistry; biology; data compilations; thermochemistry; thermodynamics.

This report is a selected and annotated bibliography of sources of data compilations relevant to biochemical thermodynamics. Included in the annotations are brief descriptions of the type of thermodynamic properties tabulated, the class of materials dealt with, and the degree of completeness of the compilations.

NBSIR 74-537. **CODATA guidelines on reporting data for chemical kinetics,** 18 pages (Aug. 1974). Order from NTIS as COM 74-11577, $4.00.

Key words: chemical kinetics; guidelines; recommended procedures for reporting data; standardization; units.

This document is a copy of the report, June 1974, of the Task Group on Data for Chemical Kinetics of the Committee on Data for Science and Technology (CODATA). In this report recommendations are made about the reporting of experimental chemical kinetics data.

NBSIR 74-543. **High temperature MHD materials,** S. J. Schneider, W. Capps, H. P. R. Frederikse, W. R. Hosler, D. A. Kauffman, E. M. Levin, C. L. McDaniel, T. Negas, and E. R. Plante, 129 pages (Aug. 1974). Order from NTIS as COM 74-11722, $5.75.

Key words: coal slag; electrical conductivity (MHD); electrodes; insulators; MHD; MHD materials; MHD materials testing; phase equilibria (MHD); vaporization (MHD); viscosity (MHD).

Under the auspices of the Office of Coal Research the National Bureau of Standards has underway a program of materials research appropriate to magnetohydrodynamics (MHD). The overall objective of the work is to provide materials property information necessary for the design, construction, and operation of an open cycle, coal fired MHD electric generation plant. The program consists of several interrelated investigations in the areas of phase equilibria, electrical properties, vaporization, viscosity and materials testing. Initial work has centered on the behavior of coal slag but also encompasses the physical and chemical characteristics of other MHD process contaminants (alkali seed) and important electrode and insulator materials. The report summarizes the important technical results obtained during the period July 1, 1972-June 30, 1974 under the combined NBS-OCR program.

NBSIR 74-544. **Kerr coefficients of nitrobenzene and water,** R. E. Hebner, Jr., R. J. Sojka, and E. C. Cassidy, 35 pages (Aug. 7, 1974). Order from NTIS as COM 74-11525, $3.00.

Key words: dielectric fluids; electrical properties of fluids; high voltage measurements; Kerr coefficient; Kerr effect; nitrobenzene; pulse measurements; water.

The Kerr coefficients of both water and nitrobenzene were measured and the variation of these quantities with temperature and wavelength was investigated. At a temperature of 296 K and at a wavelength of 632.8 nm, the following values for the Kerr coefficients were obtained $B(C_6H_5\ NO_2) = 3.24 \times 10^{-12}$ m/V^2, and $B(H_2O) = 3.43 \times 10^{-14}$ m/V^2.

The estimated uncertainty in the measurement in nitrobenzene is ± 6 percent while in water the estimated uncertainty is ± 8 percent.

The primary conclusion drawn is that although nitrobenzene can be used for accurate measurement of a wide, and fairly well defined, variety of high voltage pulses, the situation in water is more poorly understood. The primary areas of difficulty using water are the existence of turbulence under pulses of duration of a few microseconds and the possibility of a voltage dependence of the Kerr coefficient due to a saturation of the alignment of the molecules with the applied field.

NBSIR 74-545. **Notes on the fundamentals of measurement and measurement as a production process,** P. E. Pontius, 65 pages (Sept. 1974). Order from NTIS as COM 74-11656, $4.25.

Key words: calibration; comparator; interferometer; length; long gage blocks; measurement process; uncertainty.

The concept of a measurement process as a production process is relatively new, having evolved in the last ten years. There have been significant contributions from many sources which have served to refine the initial ideas. The generalized concept of a measurement process is discussed together with techniques and examples for verifying the validity of the result. While some of the techniques may not be appropriate for certain highly specialized measurement processes, it is felt that the concepts are applicable to practically all measurement processes. For certain types of general measurement processes, which must operate in a variety of environments, and which must accommodate a variety of materials and properties, the techniques have been invaluable in understanding the manner in which measurement processes operate in a "real" world.

NBSIR 74-550. **Report to AID on an NBS/AID workshop on standardization and measurement services in industrializing economies,** M. B. McNeil, 92 pages (May 11-24, 1974). Order from NTIS as COM 74-11755, $4.75.

Key words: AID; assistance; economics; foreign relations; industrializing nations; LDC's; measurement services; standardization.

On May 11-24, 1974, a Workshop was held at the National Bureau of Standards (Gaithersburg), under the sponsorship of AID, whose object was to give standards officials of industrializing nations insight into the standards and measurement systems in the United States and the role of the National Bureau of Standards, so that these officials might consider what parts of the U.S. system might usefully be adapted to conditions in their home countries. The report contains copies of speeches and presentations by representatives of both the U.S. and the industrializing nations, in addition to a general agenda of talks, presentations, and tours of laboratories both of NBS and of other organizations.

NBSIR 74-551. **An appraisal of methods for estimating self-reaction hazards,** W. Tsang and E. S. Domalski, 100 pages (June 1974). Order from NTIS as COM 74-11658, $5.25.

Key words: activation energy; bond dissociation energy; computer programs; explosive sensitivity tests; heat of decomposition; oxygen balance.

The ability to identify and specify the thermal instability of chemical substances has been appraised as a result of examining certain test methods used to measure explosive sensitivity, and certain computer programs designed to estimate reaction hazards from a thermochemical approach. The bond dissociation energy emerges as the parameter giving the best correlation with material sensitivity. The computer programs overemphasize explosive power as opposed to explosive sensitivity and label many compounds hazardous when they

are not. At present, regulations specifying the handling and transport of commodities should follow the concept of self-reactivity based upon functional groups.

NBSIR 74-552. **Technical manual for phosphor standards calibrator,** M. L. Greenough and H. K. Hammond III, 84 pages (Aug. 12, 1974). Order from NTIS as COM 74-11644, $4.75.

Key words: fluorescence measurement; instrumentation, luminescence measuring; luminescence measurement; phosphorescence measurement.

This project involved two activities, 1) the fabrication and calibration of phosphor standards for use in the Postal Service Model 4A8 Phosphoremeter and 2) the construction of an instrument to perform the calibration function. Both of these relate to standardization of the phosphorescent and fluorescent activity of the luminescent coating applied to postage stamps by the Bureau of Engraving and Printing. The purpose of the luminescent coatings is to facilitate detecting the orientation of envelopes in facer-canceler machines during mail processing.

Work on the project entailed the fabrication of approximately 60 phosphor standards, which are hand-sized aluminum blocks into which stamp-sized wafers of luminescent materials are mounted. Fabrication was carried out following the specific procedures supplied by the Postal Service, with however, authority to verify or alter the process as necessary. On the other major project effort, an instrument was designed and constructed following in general the basic design of an earlier breadboard device developed under a prior project. In the system, quantitative evaluations are ultimately referred to calibrations at NBS of the relative irradiance of a lamp in the ultraviolet and visible regions of the spectrum.

This report, one of two covering the project, is in the form of technical manual for the calibration instrument, and includes theory of operation, mechanical construction and detailed operating procedures.

NBSIR 74-564. **Development and analysis of techniques for calibration of Kerr cell pulse-voltage measuring systems VIII,** R. E. Hebner, Jr., E. C. Cassidy, and R. J. Sojka, 55 pages (Aug. 21, 1974). Order from NTIS as COM 74-11726, $4.25.

Key words: calibration; electrical measurements; high voltage measurements; insulating fluids; Kerr coefficient; nitrobenzene; pulse voltage measurement; space charge; water.

This report documents recent progress in the refinement of techniques for accurate calibration of pulsed voltage measurement based on the electro-optic Kerr effect. The work includes a discussion of calibration techniques and a comparison of calibrations performed in various laboratories. In addition the Kerr coefficients of water, nitrobenzene and Halowax oil were determined. The measurements in Halowax oil were performed under direct, 60 Hz alternating, and pulsed high voltage. The measurements of the Kerr coefficient of nitrobenzene and water were performed under pulsed high voltage, but measurements of the space charge dynamics in nitrobenzene under low frequency alternating voltage are discussed.

NBSIR 74-567. **FY 74 progress report on design criteria and methodology for construction of low-rise buildings to resist typhoons and hurricanes,** N. J. Raufaste, Jr. and R. D. Marshall, 276 pages (July 1, 1974). Order from NTIS as COM 74-11631, $3.00.

Key words: buildings; construction; data acquisition equipment; design criteria; extreme winds; information transfer; instrumentation; wind loads; wind tunnel modeling.

This report gives the major accomplishments of the second phase of a three year project to provide engineering and technical assistance to the Agency for International Development (AID), Department of State in developing improved design criteria for low-rise buildings to better resist extreme winds. During FY 74, the Center for Building Technology project staff members commenced several tasks. These tasks will serve as major inputs to the development of improved design criteria. The principal tasks include: 1) selecting a second and third field test site in the Philippines, 2) instrumenting four full scale houses, at the sites, 3) instrumenting the University of Philippines wind tunnel facility, 4) participating in an International Workshop at Manila during November 1973, and 5) developing, in conjunction with short-term consultants in Bangladesh and Jamaica, a methodology for the transfer of technology.

NBSIR 74-568. **FY 75 project plans Law Enforcement Standards Laboratory,** 62 pages (Sept. 1974). Order from NTIS as COM 74-11578, $6.25.

Key words: communications equipment; forensic science; Law Enforcement Standards Laboratory; LESL; performance standards; project plans; protective equipment; security equipment; standards.

Plans are presented for seventeen projects approved and funded for FY-75. They include plans for the preparation of performance standards, user guidelines and reports on law enforcement equipment in the communications, security, protective equipment, investigative aids, courtroom equipment and compliance testing areas.

NBSIR 74-572. **Torsional buckling of composite cylindrical shells,** D. E. Marlowe and G. F. Sushinsky, 60 pages (Sept. 1974). Order from NTIS as COM 74-11791, $4.25.

Key words: aircraft structures; buckling; composite materials; metal reinforcement; stability; stacking sequence; thin shells; torsion.

The elastic buckling strength has been determined for thin-walled composite and composite-reinforced-metal cylindrical shells. Tests were performed on boron/epoxy and graphite/epoxy-all-composite specimens, on boron/epoxy-reinforced-titanium specimens and on boron/epoxy and graphite/epoxy-reinforced aluminum specimens. Cylinders were tested with several unidirectional-ply and cross-ply layups.

The results of the tests were compared with the buckling strengths predicted by the torsional buckling analysis of Chao. For the cylinders which fail by buckling, the experimental buckling torques were approximately 81 percent of the torques predicted by the analysis.

The experimental results of tests on 39 specimens are presented. Torsional buckling strengths which differ by as much as a factor of two may result from reversing the direction of twist of a thin-walled cross-ply composite cylinder. This has been shown to be equivalent to reversing the stacking sequence of the laminate. This is of potential importance in applications where reversals of loading may occur. An "optimum" stacking sequence which produced significant increases in the predicted and measured buckling loads was determined. Cylinders fabricated with this stacking sequence exhibit considerable increases in the strength-to-weight ratio over other sequences examined.

NBSIR 74-577-1. **Remittance processing system, Volume I (Refer to Volume II),** P. D. Shupe, Jr., P. Meissner, and J. R. Park, 194 pages (Sept. 1974). Order from NTIS as COM 74-11723, $7.00.

Key words: audit trail; check endorsement; check handling; data entry; document labeling; labeling; listing; man machine interface; MICR printing; remittance processing; remittance register.

The Remittance Processing System is a prototype developed for the Internal Revenue Service to test a new concept in automating the processing of taxpayer remittances. Central to the new processing concept was the integration of the Direct Data Entry System. Initial Entry Station with equipment components that would eliminate a number of individual manual operations, permit operator interface with the central DDES computer, and provide for verification of initial entry, check endorsement, audit trail data, remittance documentation, and affixing information to taxpayer documentation accompanying the remittance. This report describes the equipment which was configured to implement these processes and to demonstrate the viability of the concept.

NBSIR 74-577-2. **Remittance processing system. Volume II (Reference Volume I),** P. D. Shupe, Jr., P. Meissner, J. R. Park, 317 pages (Sept. 1974). Order from NTIS as COM 74-11724, $9.25.

Key words: audit trail; check endorsement; check handling; data entry; document labeling; labeling; listing; man machine interface; MICR printing; remittance processing; remittance register.

The Remittance Processing System is a prototype developed for the Internal Revenue Service to test a new concept in automating the processing of taxpayer remittances. Central to the new processing concept was the integration of the Direct Data Entry System. Initial Entry Station with equipment components that would eliminate a number of individual manual operations, permit operator interface with the central DDES computer, and provide for verification of initial entry, check endorsement, audit trail data, remittance documentation, and affixing information to taxpayer documentation accompanying the remittance. This report describes the equipment which was configured to implement these processes and to demonstrate the viability of the concept.

NBSIR 74-578. **Development of microwave hygrometer model III,** D. P. Stokesberry and S. Hasegawa, 14 pages (Sept. 1974). Order from NTIS as COM 74-11765, $3.25.

Key words: dew-point; hygrometer; microwave hygrometer.

This is a progress report on the design and construction of NBS microwave hygrometer, Model III. The hygrometer is intended for field or laboratory operation with a dew point range of − 40 to 40° C.

NBSIR 74-582. **FY 1973 progress report on design criteria and methodology for construction of low-rise buildings to better resist typhoons and hurricanes,** N. J. Raufaste and R. D. Marshall, 31 pages (July 2, 1973). Order from NTIS as COM 74-11645, $3.75.

Key words: construction; design criteria; extreme winds; full-scale test buildings; housing; instrumentation; wind tunnel.

This report highlights the major accomplishments of the initial phase of a three fiscal year project to provide engineering technical assistance to the Agency for International Development (AID) for the development of design criteria for low-cost/low-rise buildings to better withstand the effects of extreme winds. This phase represents approximately a 3 month level of effort. During this period CBT project staff members commenced six introductory tasks. These tasks will set the pace for the second fiscal year level of effort. The tasks included: initiate dialogue with local organizations and institutes in developing countries, establish a local Philippine advisory committee; conduct on-site visits to developing countries to identify local professional candidates for short term consultating; conduct on-site visits to developed countries to collect information from research centers; purchase initial wind tunnel and full-scale field test instrumentation; and commence library search of related subject documents.

NBSIR 74-595. **A procedure for estimating automobile fuel consumption on congested urban roads,** D. M. Levinsohn, J. T. McQueen, 20 pages (Aug. 1974). Order from NTIS, as COM 75-10057, $3.25.

Key words: automobile fuel consumption; congestion; energy conservation; fuel consumption; impact assessment; roadway operating environment; urban roads; vehicle characteristics.

Energy consumption is an important measure of the performance of a transportation system. To be able to accurately measure associated automobile fuel consumption will improve the evaluation of urban transportation alternatives. An estimated procedure is proposed that is designed to be particularly sensitive to automible fuel consumption in congested, peak hour traffic. This procedure is based upon vehicle attributes and roadway operating conditions which were determined through an extensive review of the auto fuel consumption literature. Vehicle attributes include characteristics of the automobile that affect fuel consumption. Roadway operating conditions comprise the types of driving to which the automobiles are subjected. Vehicles are classified by weight and model year. The proposed roadway classifications are expressway, arterial, and local street. For each vehicle type category, base fuel consumption rates are determined. These base consumption rates are then modified by adjustment factors which reflect the roadway operating conditions. The rates are multiplied by the vehicle miles of each vehicle category and summed over all categories to compute the total fuel consumption on the road under analysis. An example application of the procedure including sensitivity analyses is presented. The base fuel consumption rates can be obtained from EPA emissions test data. Research is required to determine the adjustment factors, particularly under conditions of extreme roadway congestion.

This column lists all outside publications by the NBS staff, as soon after issuance as practical. For completeness, earlier references not previously reported may be included from time to time.

Arsenault, R. J., deWit, R., **Distributed glide force between a non-spherical defect and a dislocation,** *Acta Met.* **22,** 819–827 (July 1974).

Key words: Burgers vector; defect; dislocation; glide; inclusion; kink; tetragonal.

The distributed glide force on dislocations due to a ⟨100⟩ and a [110] type non-spherical defect was determined. The distributive glide force does produce a torque on a screw dislocation but it is of no consequence in terms of the effect the defect has on the nucleation of a double kink. It was also proven that the total interaction force with á non-spherical defect is indeed greater for an edge dislocation than with a screw dislocation.

Ausloos, P., Lias, S. G., **Far ultraviolet photochemistry of organic compounds,** *Proc. NATO Advance Study Institute on Chemical Spectroscopy and Photochemistry in the Vacuum Ultraviolet, Valmorin, Quebec, Canada, Aug. 5-17, 1973,* pp. 465-482 (Aug. 1973).

Key words: far ultraviolet photochemistry; free redicals; organic compounds; photofragments; primary processes; quantum yield.

A brief survey is presented concerning certain aspects of the far ultraviolet photochemistry of organic compounds. The use of spectroscopic methods and chemical analysis of final photolytic products are discussed as methods of obtaining information about the fates—particularly the modes of decomposition—of compounds excited by absorption of photons having energies above about 8 eV. Commonly used photolytic light sources which deliver photons in the energy range 7.6 eV-21.2 eV are described.

Generalizations which can be drawn concerning the primary modes of decomposition of excited alkanes, cycloalkanes, and carbonyl compounds in this energy range are discussed.

Ayres, T. R., Linsky, J. L., Shine, R. A., **Stellar model chromospheres. II. Procyon (F5 IV-V),** *Astrophys. J.* **192,** 93-107 (Aug. 15, 1974).

Key words: late-type stars; line profiles; stellar chromospheres; stellar photospheres.

We derive a model for the chromosphere and upper photosphere of Procyon (F5 IV-V) based on calibrated observations of the K and 8542 Å lines of Ca II, the k(2796 Å) line of Mg II, and the K-line wings. We demonstrate the feasibility of our model synthesis approach to derive a preliminary model chromosphere despite the lack of spatial and spectral resolution associated with solar chromospheric studies. Our upper photosphere model is very similar to the radiative equilibrium Procyon model of Strom and Kurucz, and our chromospheric model is similar to the quiet solar chromosphere temperature distribution of Shine in the 6000-8000 K range.

Bassett, D. C., Block, S., Piermarini, G. J., **A high-pressure phase of polyethylene and chain-extended growth,** *J. Appl. Phys.* **45,** No. 10, 4146-4150 (Oct. 1974).

Key words: diamond anvil pressure cell; high pressure; polyethylene; polymer; polymorphism.

Optical and x-ray observations of polyethylene have been made at high pressures and temperatures using a gasketed diamond-anvil cell. The experiments confirm the existence of the high-pressure phase previously postulated by Bassett and Turner. The new phase is hexagonal, with orthohexagonal lattice parameters of $a = 8.4_6$ Å and $b = 4.8_8$ Å. Comparison with the previously measured volume change indicates that there is a decrease in the c dimension to 2.4$_7$ Å per ethylene unit in transforming from orthorhombic to hexagonal structures. The likely implication is that the molecules in the hexagonal phase do not have an all-trans conformation. Chain-extended growth is the result of crystallization from the melt into the hexagonal phase, whereas chain-folded growth is the familiar process of melt crystallization into the orthorhombic phase. Chain-extended lamellae are observed to grow outwards behind a growing edge with a permanent narrowed profile, showing that the lamellar thickness is determined in a region extending several microns behind the growth front.

Benjamin, E. A., **A review of methods and requirements for fire protection of steel-framed buildings,** *Proc. Structural Engineering Association of California, Coronado, Calif., Oct. 3, 1968,* pp. 24-28 (1968).

Key words: building codes; E-119 test; fire protection; fire research; steel construction.

Developments in materials and techniques to meet the current building code requirements for fire protection of steel-framed buildings are described. Included is a discussion of some of the test requirements in the ASTM Standard, Methods of Fire Tests of Building Construction and Materials. Research work that may lead to improvement in the Fire Test Method is described.

Berger, M. J., **Some new transport calculations of the deposition of energy in biological materials by low-energy electrons,** *Proc. 4th Symp. on Microdosimetry, Verbania Pallanza, Italy, Sept. 1973,* pp. 695-711 (Mar. 1974).

Key words: absorbed dose distributions; electrons, delta rays and beta particles; event-size; microdosimetry; transport theory; wall effects.

After some brief remarks about the method of calculation and cross sections, illustrative results are given from recent electron transport calculations. The following topics are discussed: (1) the distribution of absorbed dose in water around point-isotropic and point-monodirectional electron sources; (2) the radial distribution of absorbed delta-ray energy around proton tracks in nitrogen; (3) the frequency mean and energy mean of microdosimetric event-size distributions in small spherical volumes in water, for the case of irradiation by electrons and tritium beta-rays; (4) the perturbation of event-size distributions in gas-filled cavities due to the presence of surrounding walls.

Blackburn, D. L., Oettinger, F. F., **Transient thermal response measurements of power transistors,** *Proc. IEEE Power Electronics Specialists Conf., Bell Telephone Laboratories, Murray Hill, N.J., June 10-12, 1974, PESC '74 Record,* pp. 140-148 (IEEE, New York, N.Y., Oct. 1, 1974).

Key words: computer simulation (transient thermal); current crowding (transistors); power transistors; thermal impedance measurements; thermal response measurements; transistors (thermal measurements).

Differences between the measured thermal impedance of power transistors when determined by the pulsed heating curve and cooling curve techniques are discussed. These differences are shown to result primarily because the power density distributions of these devices change as the devices heat; as a result of these changes the heating curve and the cooling curve are not conjugate. It is shown that the cooling curve technique, when the cooling curve is initiated from the most non-uniform steady state thermal distribution, (maximum voltage, maximum power) will indicate a larger value for the thermal impedance than will the pulsed heating curve technique, even for pulses in excess of the d-c power level. A one dimensional model for power transistor cooling is described. The theoretical predictions of the model are shown to be in good agreement for practical applications with three-dimensional computer simulations and experimental results. Using this model, it is possible to estimate an average junction temperature and the area of power generation at steady state. Both TO-66 and TO-3 encased devices of mesa and planar strucures were included in this study.

Brauer, G. M., Termini, D. J., **Grafting of monomers to collagen and hard and soft tissues,** (Proc. XXIII International Congress of Pure and Applied Chemistry, Boston, Mass., July 1971), *Macromolecular Preprint* **1,** pp. 601-608 (1971).

Key words: collagen; graft polymers; hard tissue; soft tissue; surface grafting; tissue modification.

Grafting of monomers to collagenous surfaces offers an attractive technique for modifying the surface properties of soft and hard tissues. Some 20 monomers were grafted to purified steelhide collagen powders or films using 1.10^{-3}M ceric ammonium nitrate as initiator. Yields after extraction of homopolymer were greatly dependent on the monomer used. With the most reactive monomers, surface grafts were obtained within 15 minutes. The large variety of monomers, including those with additional reactive or crosslinking groups, graftable to collagen indicates that surfaces with the desired hydrophilichydrophobic balance to fit specific applications can be otained. Some monomers such as ethylene dimethacrylate or glycidyl methacrylate could be grafted to epidermal calfskin. No apparent grafting to calfskin was observed for most of the other monomers. Apparently, the presence of the keratinous layer reduces the reactivity toward graft polymerization. On grafting glycidyl-, dimethylaminoethyl-, isobutyl methacrylate or 1,3-butylene

dimethacrylate to powdered bone, an increase in weight of from 11 percent to 60 percent after acetone and chloroform extraction was obtained. Dentin surfaces are not as susceptible to grafting as powdered bone. The relative grafting efficiency of monomers to the solid substrate decreases in the following order: collagen powder, collagen film, bone powder, epidermal calfskin, ratskin, dentin powder.

Carpenter, B. S., LaFleur, P. D., **Nitrogen determination in biological materials by the nuclear track technique,** *Anal. Chem.* **46,** No. 8, 1112-1113 (July 1974).

Key words: bovine liver, cellulose nitrate; image analyzing system; microscope; neutron activation analysis; nitrogen; orchard leaves; proton tracks; standard reference materials.

A method has been developed for the determination of nitrogen in biological matrices using the nuclear track technique (NTT). Protons from the nuclear reaction $^{14}N(n,p)^{14}C$, which is produced by thermal neutrons, leave radiation damaged trails (tracks) which are made visible to optical microscopy by chemical etching. The NTT method has been used for the analysis of leaves and liver with excellent agreement with values obtained using the Kjeldahl technique.

Clifton, J. R., Beeghly, H. F., Mathey, R. G., **Nonmetallic coatings for concrete reinforcing bars,** *FHWA-RD-74-18,* 85 pages (Available from the National Technical Information Services, Springfield, Va. 22161, Feb. 1974).

Key words: bridge decks; chloride ions; concrete; corrosion; deicing salts; epoxy coatings; organic coatings; steel reinforcing bars.

This work was undertaken to ascertain the feasibility of using organic coatings, especially epoxies, to protect the steel reinforcing bars embedded in concrete of bridge decks from rapid corrosion. This corrosion is caused by the chloride ions from the most commonly applied deicing salts, sodium chloride and calcium chloride. Altogether, 47 different coating materials were evaluated to some extent, consisting of: 21 liquid and 15 powder epoxies; 5 polyinyl chlorides; 3 polyurethanes; 1 polypropylene; 1 phenolic nitrile, and one zinc rich coating. The chemical and physical durabilities, chloride permeabilities, and protective qualities of coatings were assessed. The bonds between coated and uncoated bars and concrete were measured by both pullout and creep tests.

The results indicate that both epoxy and polyvinyl chloride coatings, if properly applied, should adequately protect steel reinforcing bars from corrosion. However, only the epoxy coated bars had acceptable bond and creep characteristics when embedded in concrete. The powder epoxy coatings overall performed better than the liquid epoxies, and four powder epoxy coatings have been identified as promising materials to be used on reinforcing bars embedded in concrete decks of experimental bridges.

Crandall, D. H., Dunn, G. H., Gallagher, A., Hummer, D. G., Kunasz, C. V., Leep, D., Taylor, P. O., **Rate coefficients for electron excitation of the first resonance transition in H, Li, Na, Ca, Ca^+, and Ba^+ calculated from experimental data,** *Astrophys. J.* **191,** No. 3, 789-793 (Aug. 1, 1974).

Key words: atomic cross sections; atomic data; atomic physics; rate coefficients; resonance lines.

By fitting cubic spines augmented with special functional forms for low and high energies to cross-section data determined experimentally at discrete values of the electron energy, we obtain an interpolation that can be visually inspected and adjusted to prevent the appearance of spurious features. The familiar integral expressing the rate coefficient in terms of the cross-sections can then be evaluated with no further approximation. This procedure is applied here to cross-section data for the first resonance transition of H, Li, Na, Ca, Ca^+, and Ba^+. The resulting collisional de-excitation rate coefficient, from which the excitation-rate coefficient can be determined by the detailed balance relation, is tabulated in each case for electron temperatures in the interval from 10^3 to 10^5 K and is expressed in terms of a Chebyshev expansion valid for this range of temperature.

Dickens, B., Prince, E., Schroeder, L. W., Jordan, T. H., **A refinement of the crystal structure of $H_3PO_4 \cdot 1/2\ H_2O$ with neutron diffraction data,** *Act. Cryst.* **B30,** Part 6, 1470-1473 (June 1974).

Key words: crystal structure; hydrates; hydrogen bonding; neutron diffraction; phosphates; phosphoric acid.

The hydrogen positions in $H_3PO_4 \cdot 1/2\ H_2O$ have been determined and the structure refined to $R_w = 0.022$, $R = 0.027$, with 1208 reflections of measurable intensity. The general features of the structure are as described by Mighell, Smith & Brown [*Acta Cryst.* (1969). **B25**, 776-781]. The two crystallographically discrete H_3PO_4 molecules are hydrogen bonded to each other and to the water molecule. The positions of the hydrogens of the water molecule appear to have been affected by H···H repulsion from the H_3PO_4 hydrogen atoms and the O_w – H···O (phosphate) hydrogen bonds are markedly non-linear. For P–O–H, the average P–O distance is 1.562 Å, the average O–H distance is 1.010 Å and the average P–O–H angle is 117°. Individual P–O–H angles range from 112.4 to 119.9°. In the water molecule, the average O–H distance is 0.997 Å, and the H–O–H angle is 106.0 (2)°. The four shortest H···H interactions range from 2.161 (3) to 2.290 (3) Å, and may imply H···H van der Waals bonding as in $Ca(OH)_2$.

Ellerbruch, D. A., **Application of measurements of electromagnetic phenomena to oceanography,** *Proc. First UJNR/MEC Symp., Record of the U.S.-Japan UJNR Joint Symp. on Marine Electronics, Tokyo, Japan, Oct. 9, 1972,* pp. 23-30 (Japanese Electrical Industrial Committee, Tokyo, Japan, 1972).

Key words: electromagnetic measurements; oceanography; sea water-return cable.

The U.S. National Bureau of Standards has developed a wide variety of measurement echniques for precisely determining the electromagnetic quantities and performance of electrical networks. Most of these measurements have been reduced to standard laboratory routines. Usually the network is transported into the laboratory, however, many measurements are utilized in the field.

The ocean can be treated as an electrical network. It is dispersive, lossy, inhomogeneous, far from a theoretically perfect medium. Nevertheless the established techniques used to evaluate laboratory sized samples of well-defined media can be used to evaluate the performance of full scale oceanic systems in situ. In those applications the measurement laboratory is transported to the network. NBS has obtained data on the performance of the multiconductor, seawater return, mooring line data line being used by the National Data Buoy Center for deploying their network of moored Environmental Buoys. A variety of measurement techniques were used in this evaluation. Data were obtained in both the time and the frequency domains.

The interaction of electromagnetic waves with the ocean provides a means for sensing and characterizing oceanic parameters. Electromagnetic sensing techniques offer interesting new approaches to the development of oceanic instrumentation. Some of these techniques will be described.

Evans, A. G., Linzer, M., Russell, L. R., **Acoustic emission and crack propagation in polycrystalline alumina,** *Mater. Sci. Eng.* **15,** 253-261 (1974).

Key words: acoustic emission; alumina; crack propagation; failure prediction; microcracking.

Acoustic emission is measured during the fracture of polycrystalline alumina. It is shown that acoustic emission is obtained during macrocrack growth, which can be used for failure indication. Acoustic emission is also obtained owing to the formation of non-

propagating grain size microcracks at the surface. This emission can mask that due to macrocrack growth, but only for short failure times or at high stresses. Models are presented which relate the acoustic emission to the various crack propagation processes.

Evans, A. G., Wiederhorn, S. M., **Proof testing of ceramic materials—an analytical basis for failure prediction,** *Int. J. Fract.* **10,** No. 3, 379-392 (Sept. 1974).

Key words: ceramics; failure probability; minimum time-to-failure; proof stress diagrams; proof testing.

An analysis is presented which permits the accurate prediction of component lifetimes after proof testing. The analysis applies to crack propagation controlled fracture but can be used as a conservative prediction when crack initiation is predominant. The analytical predictions are confirmed in a series of time-to-failure measurements.

Fano, U., Martin, W. C., **Z-dependence of spin-orbit coupling,** Paper in *Topics in Modern Physics,* W. E. Britten and H. Odabasi, Eds., pp. 147-152 (Colorado Assoc. Press, Boulder, Colo., 1970).

Key words: coupling-strength; spin-orbit coupling.

Experimental evidence on the spectroscopic spin-orbit strength parameter for p electrons, ζ_p, for neutral atoms of all atomic numbers Z is represented rather closely by the empirical formula

$$\zeta_p \, n^{*3} = 0.450 \, Z^{2.33} \text{ cm}^{-1}$$

A few comments are made regarding alternative representations of spin-orbit coupling.

Fong, J. T., **Material symmetry and scalar potentials in nonlinear theory of materials,** *Proc. Conf. on Symmetry Similarity and Group-Theoretic Methods in Mechanics, Calgary, Alberta, Canada, Aug. 19-21, 1974,* pp. 155-166 (1974).

Key words: constitutive equation; continuum mechanics; elasticity; isotropy; material symmetry; mechanical properties; rheology; scalar-potential; strain-energy; thermodynamics; viscoelasticity.

For elastic and viscoelastic materials whose constitutive equations are derivable from scalar potentials, we examine their restrictions due to (a) material symmetry alone, and (b) material symmetry plus additional physical hypothesis. New results on a class of nonlinear viscoelastic materials (Bernstein, Kearsley, and Zapas, 1963) are derived. Applications to the interpretation of experimental data on real materials are discussed.

Frederick, N. V., Stanley, W. D., Zimmerman, J. E., Dinger, R. J., **An application of superconducting quantum interference magnetometers to geophysical prospecting,** *IEEE Trans. Geosci. Electron.* **GE-12,** No. 3, 102-103 (July 1974).

Key words: geophysical prospecting; magnetometer; magnetotelluric; quantum interference; SQUID; superconductor.

Magnetotelluric field measurements were carried out at two geothermally interesting locations with two Superconducting QUantum Interference Device (SQUID) magnetometers. The tests demonstrated the very attractive combination of characteristics of these instruments for geophysical magnetic measurements. They have noise levels down to 10^{-14} T/Hz$^{1/2}$ (10^{-5} gamma Hz$^{-1/2}$); frequency response from 0 to several kHz; dynamic range of at least 160 dB; and in addition are portable and easy to set up in the field.

Frommer, M. A., Shporer, M., **The properties of water in polymeric membranes. I. Freezing and non-freezing water in cellulose acetate membranes,** *Proc. Am. Chem. Soc. 163rd Meeting on Organic Coatings and Plastics Chemistry Symp., Boston, Mass.,* **32,** No. 1, 374-381 (Apr. 1972).

Key words: cellulose acetate membranes; differential scanning calorimetry; freezing in porous systems; membranes; NMR relaxation times; nuclear magnetic resonance.

The relative amounts of freezing and non-freezing water in various water-wet cellulose acetate (CA) membranes have been determined by differential scanning calorimetry (DSC) and by nuclear magnetic resonance (NMR) techniques. DSC results suggest that: 1) A significant fraction (17-40%) of the water (1.0-3.1g H_2O per g dry CA) in any membrane does not freeze at temperatures as low as -60 °C; 2) The amount of non-freezing bound water (0.40-0.7g non-freezing water per g dry CA) depends upon the nature of the membrane, and is significantly higher than the total amount of water (all of which is non-freezing) absorbed from liquid water by a *dense* film of the same polymer ($\sim$ 0.18g water per g dry CA). The structures of the membranes studied by scanning electron microscopy suggest that the amounts of non-freezing water in cellulose acetate membranes decrease with the increase in the packing density (compactness) of the polymer within the membrane. NMR data suggest that: 3) The *non-freezing* water is *highly mobile compared with ice.* 4) The relative amounts of non-freezing water computed from NMR experiments are comparable to those estimated from DSC measurements. 5) *All* the water contained in membranes equilibrated with water vapors are bound to the polymer and do not freeze.

Gadzuk, J. W., **Electron spectroscopy of chemisorbed atoms,** (Lecture Notes from the IXth Winter School of Theoretical Physics, Karpacz, Poland, Feb. 16-29, 1972, The Theory of Metals and the Many Body Problem), *Acta Universitatis, Wratislaviensis No. 181,* **II,** pp. 1-19 (1972).

Key words: chemisorption; field emission; ion neutralization; photoemission; tunneling.

The techniques of Ion Neutralization Spectroscopy, Field Emission Resonance Tunneling and Ultraviolet Photoemission as valence level probes of chemisorbed atoms are discussed.

Grosskreutz, J. C., **Fundamental knowledge of fatigue fracture,** (Proc. Third Int. Conf. on Fracture, Munich, Germany, Apr. 8-13, 1972), Paper in *Proceedings of Third International Conference on Fracture,* pp. 1-26 (Verein Deutscher Eisenhuttenleute, Dusseldorf, Germany, Apr. 1973).

Key words: fatigue; mechanisms of fatigue; review of fatigue.

The frontiers in our knowledge of fatigue are reviewed here with the aim of describing the current status and the opportunities for fresh approaches to increase our understanding. The principal opportunity is to quantify that which we already know qualitatively. Throughout the paper an attempt is made to connect fundamental knowledge to the technical problems in fatigue which still remain vexing and unsolved.

Haar, L., Gallagher, J., **Heat capacity for gaseous ammonia,** *Proc. 6th Symp. on Thermophysical Properties, Atlanta, Ga., Aug. 6-8, 1973,* P. E. Liley, Ed., pp. 228-237 (The American Society of Mechanical Engineers, New York, N.Y., 1973).

Key words: ammonia; heat capacity; ideal gas; PVT data; PVT surface; temperature scale; thermodynamic consistency.

Several classic experiments for gaseous ammonia are shown to be thermodynamically consistent and accurate almost within their individual scatter. This feature is the basis for the extension of the range of the constant pressure heat capacity measurements (by a factor of 2 in temperature and 5 in pressure) with no appreciable loss of accuracy. For this purpose the previously calculated C_p^o values for the ideal gas are taken as bench-mark data. The real gas C_p values are tabulated for temperatures from $-30° \leq t \leq 325$ °C and pressures up to 125 bar. Over most of this range the uncertainty is several tenths percent.

Hahn, T. A., Kirby, R. K., **Thermal expansion of a borosilicate glass from 80 to 680 K—Standard Reference Material 731,** (Proc. AIP Conf. on Thermal Expansion, Lake of the Ozarks, Mo., Nov. 7-9, 1973), Paper in *AIP Conference Proceedings No. 17, Thermal Expansions, 1973,* R. E. Taylor and G. L. Denman, Eds., No. 17, 93-101 (American Institute of Physics, New York, N.Y., 1974).

Key words: borosilicate glass; dilatometer calibration; standard reference material; thermal expansion.

This Borosilicate Glass is the third Standard Reference Material (SRM) to be certified for thermal expansion measurements by the National Bureau of Standards. Copper (SRM 736) and Fused Silica (SRM 739) are the other two materials. The results of tests on six samples taken from the stock will be reported in this paper. These results indicate the stock to be of consistent quality suitable for certification. Measurements were made in the temperature range from 80 to 680 K using an interferometer apparatus. At 293 K the expansivity is $4.78 \times 10^{-6}\,K^{-1}$ and the standard deviation is $0.06 \times 10^{-6}\,K^{-1}$ calculated from a least squares fit to the data over the entire temperature range. A description of the calibration of a fused quartz dilatometer using the three Standard Reference Materials will also be presented.

Hall, J. L., **Sub Doppler spectroscopy, methane hyperfine spectroscopy, and the ultimate resolution limits,** *Proc. Aussois Conf. on Spectroscopy Without Doppler Broadening, Aussois, France, May 1973,* pp. 105-125 (1973).

Key words: laser spectroscopy; methane; molecular hyperfine spectra; saturated absorption spectroscopy; ultrahigh resolution.

The most recent results on saturated absorption spectroscopy of methane are presented. 2nd order Doppler shift and photon recoil shift are shown to be some of the limiting factors of this technique.

Harrison, C. A., **Utilization of cation-selective membranes in the study of caries formation,** *J. Dent. Res.* **53,** Suppl. to No. 5, 1023-1032 (1974).

Key words: activity; calcium hydroxide; dental caries; mechanism; permselective membrane.

A caries mechanism was tested in a model experiment in which cation-permselective membranes were used to simulate the outer enamel-plaque layer. According to this theory, preferential diffusion of Ca^{2+} and H^+ accelerates caries formation. The results support the theory and confirm that activity of $Ca(OH)_2$ is of fundamental importance.

Harrison, J. O., Jr., **New information processing standards,** (Proc. of the American Association of State Highway Officials Committee on Electronics National Conf., Seattle, Washington, May 6-7, 1969), Paper in *Committee on Electronics,* pp. 23-35 (1969).

Key words: Cobol; computers; information interchange; information processing; standards.

Information processing standards are needed for the interchange of machine sensible data, the interchange of computer programs, the interchange of computer components and devices, and the interchange of computer related ideas among people. Organizations for the development of such standards exist at four levels: international, national, Federal Government, and State Government. Two important standards recently adopted are the United States of America Standard Code for Information Interchange and United States of America Standard COBOL. Federal information processing standards are promulgated through the Federal Information Processing Standards Register.

Harvey, D. G., Achenbach, P. R., **Opportunities for improving energy utilization in residences,** *Proc. Effective Energy Utilization Symp., Drexel Univ., Phila., Pa., June 8-9, 1972,* pp. 234-247 (1972).

Key words: appliance performance; energy conservation; energy use; heating and air conditioning; residential energy consumption.

The construction features of a typical single-family residence in the northeast region of the United States are described together with average annual energy consumption for space heating and cooling, domestic water heating, and electric appliances. The market saturation in the use of the various electrical appliances in the typical residence is summarized. The potential for energy savings in the design and use of appliances, heating, ventilating, and air conditioning systems, and the building itself is summarized with reference to cost effectiveness and acceptability to the occupant. A summary of recommended areas for research in energy conservation in residences is provided.

Henderson, M. M., **Programs and services of the Federal Library Committee's task force on automation,** *Proc. 1st Annual Federal Interagency Field Librarians' Workshop, Washington, D.C., Sept. 24-28, 1972,* pp. 57-68 (Sept. 1972).

Key words: automation of library operations; Federal Library Committee; field libraries; library automation; task force on automation; FLC.

The Federal Library Committee's Task Force on Automation (TFA) has established a program which will contribute to effective and efficient improvement of Federal library and information services. The program is based on data collected during a recent survey of the Federal library community, for which the TFA served in a technical advisory capacity. Priorities include development of a tutorial workshop on techniques of evaluation for library automation, establishment of a reference file on current Federal library automation activities, and participation in a study of the feasibility of a Federal library service center operation. Such programs are of interest, and will prove of benefit, to field libraries within the Federal establishment.

Hill, J. E., Furlong, R. R., **ASHRAE cooling load calculation,** *ASHRAE J.,* pp. 61-66 (May 1973).

Key words: ASHRAE handbook; cooling load; equivalent temperature differentials; heat gain.

An attempt has been made to give an overview of the changes in the cooling load calculation methodology as appears in Part 1, Chapter 22 of the 1972 ASHRAE Handbook of Fundamentals. The distinction between heat gain, cooling load and heat extraction rate is made. The basis for calculating an instantaneous rate of heat gain for a space is given. Particular emphasis is given to the component of gain that occurs through exterior walls and roofs. The tables of equivalent temperature differentials that appear in the chapter are completely changed from those that appear in the 1967 edition. The way the values of TETD were calculated and are intended to be used are explained. In addition, the procedure of converting an instantaneous rate of total heat gain to an instantaneous space cooling load (as outlined in Part 1, Chapter 22) is explained and discussed in reference to other methods currently in use.

Hill, J. E., Kusuda, T., Powell, F. J., **A concept for determining the need for air conditioning,** (Proc. ASHRAE Symp. for Air Conditioning Criteria for Man's Living Environment, Louisville, Ky., June 24-28, 1973), *ASHRAE Bull. LO-73-8,* pp. 14-17 (1973).

Key words: air conditioning criteria; comfort indices; human comfort.

Previously written criteria that govern the decision to install or not to install air conditioning, have been based solely on the climate. This paper proposes the need for a criteria with a sounder technical base together with the manner in which it can be established. Detailed building data and hour by hour weather data are combined in a precise thermal simulation to predict the hour by hour indoor condi-

tions that would exist (dry-bulb temperature, wet-bulb temperature, and mean radiant temperature). The conditions are in turn compared to the accepted comfort standards (ET*, Kansas State University Index, Predicted Mean Vote, etc.) in order to ascertain whether air conditioning is required.

The paper gives the details of a comprehensive study showing the feasibility of such a scheme. A thermal simulation was made on an apartment building located in Jersey City, New Jersey, using the weather data of ten consecutive summers. The simulation results revealed the extent and duration of undesirable indoor conditions when this apartment is not air-conditioned. The magnitude of computational effort appears formidable if detailed simulation calculations are to be carried out for the many combinations of buildings and climatic zones in the United States. Therefore, an attempt was made to obtain statistical correlations between the indoor and outdoor conditions for this apartment. The attempt was reasonably successful and a short-cut technique for establishing criteria is indicated.

Hilsenrath, J., **Input techniques for technical information,** *Proc. Forum of Federally Supported Information Analysis Centers, NBS, Gaithersburg, Md., May 17-18, 1971*, pp. 71-88 (Available as PB208-018 from the National Technical Information Service, Springfield, Va. 22161, Jan. 1972).

Key words: computer-assisted printing; computer input; electronic typesetting; input techniques; keyboarding conventions; phototypesetting; text automation.

A summary is presented of recent progress at NBS in the automation of book production through the development of techniques for computer-assisted phototypesetting. The strength of the system rests on general-purpose edit-insertion programs and other general-purpose programs which accept a variety of input media. The programs take existing files on punched cards or computer tapes; or Magnetic Tape Selectric Typerwriter (MTST) cartridges; or files keyboarded on-line to a time-shared text editing system; and transform them to match the requirements of the phototypesetting system at the U.S. Government Printing Office (GPO).

Examples are shown of finished text consisting of upper and lower case Roman and Greek characters, subscripts and superscripts keyboarded on a variety of input devices. The examples are from input on punched cards, from a 44 key Selectric terminal and from a "scripting" teleprinter capable of typing 126 characters in two colors in inferior, superior or main line positions.

Hoer, C. A., **The 6-port coupler; a new approach to measuring V, I, P, Z, and θ, (Summary),** (Proc. Conf. Digest on Precision Electromagnetic Measurements, Boulder, Colo., June 26-29, 1972), *CPEM Digest*, pp. 15-17 (1972).

Key words: current; directional coupler; impedance; phase; power; voltage.

A 6-port coupler is described having four side arms whose outputs are proportional to the voltage, current, incident voltage wave, and reflected voltage wave at some desired measurement plane in the transmission line. The phase relationship between the outputs is the same as between corresponding quantities at the measurement plane. Complex impedance and phase angle as well as voltage, current, and power can be obtained from simple power or voltage magnitude measurements at the four side arms.

Hord, J., **Cavitation in liquid cryogens. IV. Combined correlations for venturi, hydrofoil, ogives, and pumps,** *NASA CR-244B*, 103 pages (National Aeronautics and Space Administration, Washington, D.C., Oct. 1974).

Key words: cavitation; cryogenics; hydrofoil; impellers; inducers; ogives; pumps; venturi.

This is the fourth and final volume on the results of a series of experimental and analytical cavitation studies. Previous volumes contain basic analyses and experimental data for a venturi, a hydrofoil, and three scaled ogives. Cross-correlation of the developed cavity data for these five hydrodynamic bodies is performed in this report. The data, for liquid hydrogen and liquid nitrogen, are correlated by using the extended theory derived in Volume II (CR-2156). The new correlating parameter, MTWO, improves data correlation for these stationary bodies and for pumping equipment. The results of this study are applied to the cavitating pump impeller and inducer data published by the NASA Lewis Research Center. Existing techniques for predicting the cavitating performance of pumping machinery are extended to include variations in flow coefficient, cavitation parameter, and equipment geometry. The new predictive formulations hold promise as a design tool and universal method for correlating pumping machinery performance. Application of these predictive formulas requires prescribed cavitation test data or an independent method of estimating the cavitation parameter for each pump. The latter would permit prediction of performance without testing; potential methods for evaluating the cavitation parameter prior to testing are suggested. Directions for future work are indicated.

Huebner, R. H., Celotta, R. J., Mielczarek, S. R., Kuyatt, C. E., **Oscillator strength values derived from electron energy loss spectra of molecules,** (Proc. VIII Int. Conf. on the Physics of Electronic and Atomic Collisions, Beograd, Yugoslavia, July 16-19, 1973), Abstracts of Papers of the *VIII International Conference on the Physics of Electronic and Atomic Collisions*, B. C. Cobic and M. V. Kurepa, Eds., **I** 435-436 (Institute of Physics, Beograd, Yugoslavia, May 1973).

Key words: acetone; energy loss spectra; ethanol; methanol; oscillator strengths.

The method of obtaining oscillator strengths from electron energy loss data is described.

Isler, M. A., Stenbakken, G. N., **Mechanically actuated switches for burglar alarm systems,** *NILECJ-STD-0302.00*, 18 pages (U.S. Department of Justice, Law Enforcement Assistance Administration, National Institute of Law Enforcement and Criminal Justice, Washington, D.C., May 1974).

Key words: burglar alarm sensor; burglar alarm system; door switch; mechanically actuated switch; perimeter sensor; switch.

This standard establishes performance criteria for mechanically-actuated electrical switches intended for use in protective intrusion alarm circuits to monitor the position of doors, windows, etc. These devices cause the initiation of an alarm signal to a police panel, central station, or local audible alarm device. Included are requirements and test methods for performance, electrical properties and materials. The performance characteristics addressed are those that affect the false alarm susceptibility of the device. This standard does not provide performance criteria for the ability of these devices to resist attempts to defeat them through physical or surreptitious attack.

Johnson, D. R., Kirchhoff, W. H., **Centrifugal distortion and predictability in the microwave spectrum of formamide,** (Proc. Symp. on Interstellar Molecules, Charlottesville, Va., Oct. 4-5, 1971), Paper in *Molecules in the Galactic Environment*, M. A. Gordon and L. E. Snyder, Eds., pp. 247-253 (John Wiley and Sons, New York, N.Y., 1973).

Key words: centrifugal distortion; critical review; formamide; interstellar molecules; microwave spectra.

Recent detection of emission signals from interstellar formamide (NH_2COH) has stimulated a renewed interest in the laboratory microwave spectrum of this molecule. Previous laboratory investigations of formamide were aimed primarily at obtaining structural parameters and other related information. The spectral observations reported in these early papers have much in common with the available literature on other interstellar molecules. Reported transitions either do not include those accessible to the radio telescopes or were

not measured with sufficient resolution to be useful for a positive molecular identification.

The present paper describes a detailed investigation of the effects of centrifugal distortion and nuclear quadrupole hyperfine splitting on the microwave spectrum of formamide. Molecular parameters obtained from this investigation have been used to predict the entire rotational spectrum of $^{14}NH_2$ $^{12}C^{16}OH$ potentially accessible to the telescopes. The procedures illustrated with formamide may be applied to other molecules to predict interstellar transitions which are difficult to measure in the laboratory.

Julienne, P. S., Krauss, M., **Molecule formation by inverse predissociation,** (Proc. Symp. on Interstellar Molecules, Charlottesville, Va., Nov. 4-7, 1971), Paper in *Molecules in the Galactic Environment*, M. A. Gordon and L. E. Snyder, Eds., pp. 354-373 (John Wiley and Sons, New York, N.Y., 1973).

Key words: Bates mechanism; Feshbach-type resonance states; inverse predissociation; molecule formation; non-adiabatic interactions; radiative association; two-body recombination rates.

One of the dominant mechanisms for interstellar molecule production has long been thought to be radiative association. We wish to broaden the usual understanding of this process and present a theory for molecule formation through inverse predissociation which must be considered along with the Bates mechanism as being important under interstellar conditions. Although molecule formation by a two-body collision can occur only upon continuum to bound radiation, we will demonstrate that the presence of Feshbach-type resonance states embedded in the continuum must be considered. Thus, two colliding ground state atoms may populate excited bound molecular electronic states which radiate to produce a stable molecule. This mechanism can be operative in molecules for which the direct continuum emission of the Bates mechanism is not possible. We have calculated the two-body recombination rate constant for OH to be $\sim 3 \times 10^{-20}$ cm^3 sec^{-1} above around 20 K. This rate results from the mixing of OH $A^2\Sigma^+$ $v=1$ bound levels with the ground $X^2\Pi_{3/2}$ continuum by virtue of the breakdown of the Born-Oppenheimer approximation. Preliminary calculations for two-body recombination rates for other molecules indicate that CH, CN, and NO can also be formed through intermediate resonance states with rates exceeding 10^{-18} cm^3 sec^{-1} at low temperatures. We will present a general theory of radiative association by inverse predissociation, including (1) the scattering formalism for the calculation of the Einstein A coefficient, (2) a classification of the various couplings which are possible, together with simple rules for deciding when they may be important, and (3) results of calculations for the formation rates of specific molecules.

Kaldor, A., Braun, W., Kurylo, M. J., **Infrared laser enhanced reactions: $O_3 + SO$,** *J. Chem. Phys.* **61,** No. 7, 2496-2499 (Oct. 1, 1974).

Key words: apparatus and methods; chemiluminescence; emission spectra; free radicals; kinetics of reactions; lasers, infrared;

Vibrationally excited ozone, O_3, produced by CO_2 laser radiation was found to react with SO significantly faster than thermal ozone via the chemiluminescent reaction process $O_3 + SO \rightarrow SO_2(^1B_1) + O_2(^3\Sigma_g)$. The vibrational rate enhancement of this reaction was 2.5 ± 0.6 at 300 K. This represents the utilization of 27 percent of the available vibrational energy to promote the reaction based on a model assuming involvement of a single vibrational mode. The laser enhanced chemiluminescence measured from 260 to 450 nm was found to exhibit a 630 ± 200 cm^{-1} blue shift. This is interpreted as a partitioning of the available vibrational energy of O_3 in the vibrational manifold of the $SO_2(^1B_1)$ product.

Keplinger, M. S., **The case for the invisible copies,** *Rev. Int. Droit Auteur*, pp. 2-31 (1971).

Key words: computers; copyright; information storage and retrieval; infringement; input; intellectual property; law.

The problem of control of the use of copyrighted works in computerized information storage and retrieval systems is discussed. It is concluded that such input may be considered copyright infringement under the current Copyright Revision Bill as interpreted through the teachings of recent court decisions, as well as being an infringement under the current copyright statute. Since the input of this material may be assumed to be infringement, a method for control of the author's right must be devised to protect the author and provide for efficient dissemination of the information. To aid in this control a clearinghouse for copyright concept is suggested.

Kessler, E. G., Jr., **Determination of the Rydberg constant from the He II $n = 3 - 4$ (4686 Å) line complex,** (Proc. Fourth Int. Conf. on Atomic Masses and Fundamental Constants, Teddington, England, Sept. 1971), Paper in *Atomic Masses and Fundamental Constants*, J. H. Sanders and A. H. Wapstra, Eds., pp. 427-434 (Plenum Press, London, England, 1972).

Key words: fine structure; helium; Rydberg constant.

Absolute wavelength measurements of some of the fine structure components of the He II transition at 4686 Å ($n = 3 - 4$) are being measured to establish a new value for the Rydberg constant. The He II transition is excited in a cooled-hollow-cathode discharge and is resolved and compared to a standard source by use of a pressure-scanned double Fabry-Perot spectrometer. Problems associated with precision wavelength measurements using pressure-scanned interferometers will also be discussed.

Kirchhoff, W. H., **Determination of force fields by analysis of centrifugal distortion in microwave spectra,** (Proc. Conf. Critical Evaluation of Chemical and Physical Structural Information, Dartmouth College, Hanover, N.H., June 24-29, 1973), Paper in *Critical Evaluation of Chemical and Physical Structural Information*, D. R. Lide, Jr., and M. A. Paul, Eds., pp. 312-322 1974).

Key words: centrifugal distortion; force field; microwave spectra.

This paper describes the accuracy of molecular force fields derived from centrifugal distortion constants. Only bent, symmetric, triatomic molecules are discussed. The discussion deals primarily with the discrimination between the effects of measurement and model errors. The accuracy of the force field is judged by calculating from the force constants of the harmonic, fundamental vibrational frequencies and comparing these with the harmonic frequencies obtained from the infrared spectrum. This comparison, in turn, is measured against measurement errors arising from a statistical analysis of the microwave spectra. The particular molecular species for which such an analysis has been performed are SO_2, OF_2, SiF_2, O_3, OCl_2, CF_2, and SF_2.

Kirsch, R. A., **Resynthesis of biological images from tree-structured decomposition data,** (Proc. Int. Federation on Information Processing, Vancouver, British Columbia, May 22-26, 1972), Chapter in *Graphic Languages*, F. Nake and A. Rosenfeld, Eds., pp. 1-19 (North-Holland Publ. Co., Amsterdam, The Netherlands, 1972).

Key words: biomedical; image processing; pattern recognition.

In this paper we are simultaneously concerned with methods for decomposing grey scale microscope images and with methods for verifying the correctness of these decompositions. One such method is resynthesis. Resynthesis is viewed as a procedure whereby an analyzed scene can be reconstituted and subjected to an analysis by human (informal) methods to determine the information preservation of the process. Several algorithms are presented for different ways of resynthesizing a decomposed image from its morphological decomposition analysis.

Klein, G. P., Hamilton, C. A., **Measure power with a calculator chip and a DPM. By direct multiplication of current and voltage, you can cover a dynamic range of almost seven decades,** *Electron. Des.* **21,** 112-114 (Oct. 11, 1974).

Key words: calculator chip; digital panel meter; laser power.

This paper discusses techniques used in developing a direct reading laser power meter. Minimum modifications to a digital panel meter and the proper interfacing with a decimal arithmetic processor make this task possible. Actual working models of this device along with the power detectors are presently in use within NBS.

Klein, R., **Gas-solid interactions: Laboratory paradigms for reactions on interstellar grains,** (Proc. Conf. on Interstellar Molecules, Charlottesville, Va., Oct. 4-5, 1971), Paper in *Molecules in the Galactic Environment,* M. A. Gordon and L. E. Snyder, Eds., pp. 390-398 (John Wiley and Sons, New York, N.Y., 1973).

Key words: interstellar molecules; low temperature chemistry; surface reactions.

Reactions observed at temperatures below 150 K include those of atomic hydrogen and atomic oxygen in their ground electronic states interacting with condensed olefinic hydrocarbons. These serve as models for consideration of reactions on interstellar grains. The atomic hydrogen adds to the olefin on the surface with the resultant alkyl radicals diffusing into the interior and reacting further. Atomic oxygen diffuses into and reacts in the condensed volume. These reactions are discussed in terms of molecule formation. It is noted that the activation energy barriers are sufficiently high, both for reaction and diffusion, that it is unlikely that these reactions may serve as useful models for molecular syntheses in the H-I region.

Kruger, J., Hayfield, P. C. S., **Ellipsometry in corrosion testing,** (Proc. Symp. on State-of-the Art of Corrosion Testing, Toronto, Canada, June 21-27, 1970), Chapter 32 in *Handbook on Corrosion Testing and Evaluation,* W. H. Ailor, Ed., pp. 783-831 (John Wiley & Sons, New York, N.Y., 1971).

Key words: corrosion; electrochemistry; ellipsometry; oxidation; thickness measurements.

Because corrosion processes are strongly affected by the presence of thin films, the optical technique of ellipsometry which measures the thickness of these films and their optical properties is a valuable tool for corrosion research and testing. This technique measures the change in the state of polarization upon reflection of polarized light from a metal surface and relates these changes to the thickness and refractive index of films formed on this surface while it is immersed in an aqueous solution or in gaseous environments. Since experimentally the technique only requires that one provide a means for light to be reflected from a passive or corroding surface, it can be combined with electrochemical or diffraction techniques.

Numerous examples of ways in which ellipsometry can be applied to corrosion science and engineering measurements of film formation and dissolution kinetics and changes in film and metal surface properties are described.

Lafferty, W. J., **Determination of potential functions and barriers to planarity for the ring-puckering vibrations of four-membered ring molecules,** (Proc. Conf. Critical Evaluation of Chemical and Physical Structural Information, Dartmouth College, Hanover, N.H., June 24-29, 1973), Paper in *Critical Evaluation of Chemical and Physical Structural Information,* D. R. Lide, Jr., and M. A. Paul, Eds., pp. 386-409 (National Academy of Sciences, Washington, D.C., 1974).

Key words: barrier heights; four-member ring molecules; infrared spectroscopy; microwave spectroscopy; Raman spectroscopy; ring-puckering.

Experimental and model errors in the determination of barrier heights in four-membered ring molecules are discussed.

LaFleur, P. D., **Biological matrix standard reference materials for trace element determinations,** (Proc. Int. Conf. on Modern Trends in Activation Analysis in Saclay, France, Oct. 2-6, 1972), *J. Radioanal. Chem.* **19,** 227-232 (1974).

Key words: biological; bovine liver; orchard leaves; standard reference materials; trace elements.

Two new biological matrix Standard Reference Materials, SRM-1571, Orchard Leaves and SRM-1577, Bovine Liver, have been issued by the United States National Bureau of Standards. The content of a number of trace elements has been certified in these materials. The preparation and analytical program of the standards is described; these materials should be of great value in assuring quality control and in developing new procedures for analysis of biological materials.

Laufer, A. H., Bass, A. M., **Rate constants for reactions of methylene with carbon monoxide, oxygen, nitric oxide, and acetylene,** *J. Phys. Chem.* **78,** No. 14, 1344-1348 (1974).

Key words: inorganics; methylene; radical; rate constant; singlet; triplet.

Rate constants for some reactions of triplet and singlet methylene have been measured by means of the flash photolysis of ketene with product analysis by gas chromatography. Rate constants for reactions of triplet methylene with NO, O_2, and C_2H_2 in helium are $1.6 \pm 0.1 \times 10^{-11}$, $1.5 \pm 0.1 \times 10^{-12}$, and $7.5 \pm 1.0 \times 10^{-12}$ cm^3 molecule^{-1} sec^{-1}, respectively, over the pressure range of at least 50-700 torr. The rate constant of triplet CH_2 with CO in 700 torr of helium was $\leq 1.0 \times 10^{-15}$ cm^3 molecule^{-1} sec^{-1}. Rate constants for reaction of singlet CH_2 with NO, O_2, CO, and CH_2CO were $< 4 \times 10^{-11}$, $< 3 \times 10^{-11}$, $< 9 \times 10^{-12}$, and $3.2 \pm 1.2 \times 10^{-11}$ cm^3 molecule^{-1} sec^{-1}, respectively. The triplet CH_2 reactions were measured relative to $^3CH_2 + {}^3CH_2 \rightarrow C_2H_2 + (H_2 \text{ or } 2H)$. The rate constants for singlet CH_2 were relative to $^1CH_2 + He \rightarrow {}^3CH_2 + He$.

Lauritzen, J. I., Jr., Zwanzig, R., **Dielectric relaxation of a single axis rotator with two equivalent sites,** *Advan. Mol. Relaxation Processes* **5,** 339-361 (1973).

Key words: dielectric loss; relaxation; single axis rotator; site model; Smoluchowski's equation.

The dielectric relaxation of a single axis rotator subject to a sinusoidal potential due to the crystalline field has been calculated for a polycrystalline sample, assuming the relaxation of the dipolar orientation is governed by Smoluchowski's equation. For large values of the potential barrier the dielectric loss corresponds to that due to a two site model. For intermediate values of the potential barrier the dielectric loss corresponds to two slightly broadened Debye loss curves which may be sufficiently separated to be bimodal.

Leasure, W. A., Jr., Bender, E. K., **Tire-road interaction noise,** *Proc. Inter-Noise 73 Conf., Copenhagen, Denmark, Aug. 22-24, 1973,* pp. 421-425 (1973).

Key words: acoustics; noise (sound); tire noise; transportation noise.

The relative importance of tire noise to overall vehicle noise is established. A general description is then given of the tire engineering process and of tire structures. The important parameters influencing tire noise are discussed, based on presently-available data, followed by an identification of unknown and contradictory areas. The basic mechanisms of tire-noise generation, although not well understood, are investigated largely from a theoretical viewpoint. Areas for future research and development are identified based on gaps in the existing physical data base and a rather primitive level of understanding of noise-generating mechanisms.

Leasure, W. A., Jr., Mathews, D. E., Rinkinen, W. J., **Truck Noise 1-A: Noise evaluation tests of military truck tires,** *Report No. DOT-TST-74-21,* 53 pages (Available as PB234-348 from the Na-

tional Technical Information Service, Springfield, Va. 22161, Feb. 1974).

Key words: acoustics; noise measurement; noise(sound); tire noise; transportation noise; trucks.

This report presents the A-weighted sound level and one-third octave band spectral data resulting from a study conducted to characterize the noise generated by military truck tires. The study was conducted by the National Bureau of Standards in cooperation with the U.S. Department of Transportation under the sponsorship of the U.S. Army Tank-Automotive Command. The data base established will allow for comparison of the tire noise generated by military and commercial truck tires.

The study investigated the influence of load and speed on the noise generated by tires with four different tread designs: the standard Army tire, a retread of Army design and commercial tires with rib and cross-bar type tread patterns. Army and commercial trucks were utilized as test vehicles.

In addition, the report includes a discussion of the measurement and analysis techniques utilized for the establishment of this data base.

Lechner, J. A., **Effective statistical tests for detection models,** *Proc. 30th Military Operations Research Symp., Ft. Lee, Va., Dec. 12-14, 1972*, pp. 1-26 (1972).

Key words: detection models; detections; generalized Poisson process; statistical tests; testing.

A "Detection Model" is an entity which calculates an instantaneous probability of detection of a "target" by a "hunter," from the values of variables which describe the environment and the actions of both hunter and target, including past history, if appropriate. Given such a model, and a succession of non-identical trials which terminate at detection or after a given period of time (whichever occurs first), it is desired to test the adequacy of the model.

An approach to this problem is presented, based upon recognizing the set of trials as a nonhomogeneous Poisson process. Ways to improve the "power" of such tests by rearranging various segments of the trials are presented and discussed, including proper implementation of the tests using a digital computer. Extensions to the problem of improving the model and/or devising a new model are briefly discussed.

Leep, D., Gallagher, A., **Electron excitation of the lithium 6708-Å resonance line,** *Phys. Rev. A* **10,** No. 4, 1082-1090 (Oct. 1974).

Key words: electron excitation; lithium.

We have measured the relative optical excitation function and the polarization of the 6708-Å line, using crossed beams of electrons and lithium-6, for electron energies from threshold to 1400 eV. The electron energy resolution was ~ 0.25 eV, and the lithium-beam optical depth was small and varied. We have normalized our excitation function to Born theory at 1404 eV, where the energy dependence has converged to the theoretical behavior. Between 2 and 6 eV, the measured cross section is (10-45) percent smaller than the results of the most recent close-coupling calculations, but the measured polarization P agrees with these theories within 20 percent of P. The theoretical polarization at threshold is not observed with our energy resolution.

Levine, J., **Precision long-path interferometry and its application to geophysics and astrophysics,** (Proc. Conf. Digest on Precision Electromagnetic Measurements, Boulder, Colo., June 26-29, 1972), *CPEM Digest*, p. 115 (1972).

Key words: geophysics; interferometry; saturated absorption stabilizer; strainmeter.

We are currently operating a 30-meter Fabry-Perot interferometer as a strainmeter in an unworked gold mine near Boulder, Colorado. The interferometer is illuminated by a 3.39 μm single mode helium-neon laser. The laser is locked to one of the transmission maxima of the Fabry-Perot by means of a servo loop which tunes the laser so as to maximize the power transmitted through the long path. The tuning is accomplished by mounting one of the laser mirrors on a piezoelectric ceramic and by applying a suitable voltage to the ceramic.

Lide, D. R., Jr., **The XYZ's of laboratory frequency measurements,** Chapter in *Molecules in the Galactic Environment*, M. A. Gordon and L. E. Snyder, Eds., pp. 234-245 (John Wiley & Sons, New York, N.Y., 1973).

Key words: gaseous molecules; interstellar absorption lines, microwave absorption lines; microwave spectroscopic data.

The techniques of laboratory measurement of microwave absorption lines of gaseous molecules are reviewed. The various contributions to line widths are discussed with respect to their influence on the accuracy of typical frequency measurements reported in the literature. The reliability of calculated frequencies is discussed, as well as the general problem of identifying interstellar absorption lines on the basis of coincidences with tabulated laboratory frequencies. Useful sources of microwave spectroscopic data are summarized.

Lindamood, G. E., **A collection of mathemusicals,** *J. Irreproducible Results* **20,** No. 1, 30 (June 1973).

Key words: humor.

This article is an attempt at mathematically-oriented humor of the sort which occasionally appears in *Mathematics Magazine*. It consists of a list of titles of musical comedies, altered to suggest some mathematical concept, suggested by a fictitious professor to whom similar mathematical whimsy has been attributed in the literature.

Little, J. L., **Impact of the ASCII code and printing devices on conventions for alphanumeric display terminals: Part 1,** *Commun. Soc.* **10,** No. 1, 7-10 (Mar. 1973); **10,** No. 2, 6-11 (May 1973).

Key words: alphanumeric displays; ASCII Code; cathode-ray-tube displays; control functions; display terminals; interactive terminals; remote computer terminals; soft copy; test editing displays; user control functions; visual displays.

This paper reviews briefly the evolution of the American Standard Code for Information Interchange (ASCII) and its international version (ISO R-646). It also reviews the evolutionary impact of typewriters, teletypewriters, and the ASCII code on conventions now employed in alphanumeric display terminals. It shows a proposed keyboard layout, some approved graphic subsets of ASCII, and some codes used in computers. Current developments in the representation of extended versions of ASCII in 7 and 8 bits are given. Proposed code assignments of control functions for alphanumeric display terminals are also included, with a warning that their standardization is under the jurisdiction of the American National Standards Institute's Technical Committee X3L2 on Character Codes.

Locke, J. W., **Data limitations for the prediction of dangerousness,** (Proc. Conf. on Preventive Detention Center for Continuing Education, University of Chicago, Chicago, Ill., Oct. 28-30, 1969), Paper in *Preventive Retention*, pp. 117-131 (Urban Research Corp., Chicago, Ill., 1969).

Key words: bail; criminal justice; dangerousness; data collection; prediction; statistical analysis.

Statistical data used in past studies to describe criminal activity of people while on pre-trial release have been questioned by many familiar with the Criminal Justice System because of their limited scope. This paper describes some of the problems associated with the development of a substantially broader data base. It also includes a

discussion of incompleteness, inaccuracy and other inadequacies of available court data for developing methods of predicting dangerousness of individuals who enter the Criminal Justice System. Brief reference is made to dangerousness criteria and to prediction techniques which may have application in deciding whether or not to elease defendants before trial. The discussion is based upon the early stages of a pilot study being conducted for the National Institute of Law Enforcement and Criminal Justice.

Loevinger, R., **Absorbed dose from interstitial and intracavitary sources,** (Proc. Conf. Afterloading in Radiotherapy, New York, N.Y., May 6-8, 1971), Chapter in *Afterloading in Radiotherapy*, N. Simon, Ed., DHEW Publ. (FDA) 72-8024 BRH/DMRE 72-4, pp. 192-203 (U.S. Department of Health, Education, and Welfare, Bureau of Radiological Health, Rockville, Md. 20852, Dec. 1971).

Key words: absorbed dose; buildup factor; gamma radiation; implant; interstitial; intracavitary; point source.

A quantity of importance in the dosimetry of γ-ray sources is the ratio of the absorbed dose to the exposure in air at the same point. This is calculated from energy-absorption buildup factors for some γ-ray sources of clinical importance, and shows reasonable agreement with formulae which represent experimental determination. It is shown that penetration through tissue is adequate for implant therapy for quantum energies as low as 25 keV.

Loevinger, R., **Some remarks on the MIRD Schema for absorbed-dose calculations for biologically-distributed radionuclides,** (Proc. Symp. on Medical Radionuclides: Radiation Dose and Effects, Oak Ridge, Tenn., Dec. 8-11, 1969), Chapter in *Medical Radionuclides: Radiation Dose and Effects*, R. J. Cloutier, C. L. Edwards, W. S. Snyder, Eds., pp. 481-489 (Available as CONF-691212 from the National Technical Information Service, Springfield, Va. 22161, June 1970).

Key words: dosimetry, radionuclide; internal dose calculation; nuclear medicine; radionuclide dosimetry; reciprocity relationship; specific absorbed fraction.

The origin of the MIRD Schema [*Journal of Nuclear Medicine*, Supplement No. 1 (February 1968)] is described. The basic concepts, equations, and advantages are discussed and explained. The concept of specific absorbed fraction allows formulation of a single equation that covers internal-dose calculations for all radiations, sources and targets.

Mabie, C. P., **Adhesive refractory protective coating for investment casting,** *J. Dent. Res.* **53,** No. 5, 1181-1188 (Sept.-Oct. 1974).

Key words: casting; coat; dental; investment; refractory.

A refractory protective coat has been developed that greatly reduces scale formation and is capable of lowering sandblasted casting roughness 30 to 50 percent. When applied as a thin film to the refractory model, it remains as a tacky base which will fix wax and plastic.

Madden, R. P., **Absolute detectors and the transfer standard problem in the vacuum ultraviolet,** *Proc. Calibration Methods in the Ultraviolet and X-Ray Regions of the Spectrum Symp., Munich, Germany, May 1968,* pp. 111-124 (European Space Research Organization, Munich, Germany, 1968).

Key words: anodized aluminum; chromium; gold; photoelectric yield; radiometric standards; rare gas ionization chamber; thermopiles; tungsten; vacuim ultraviolet.

Thermopiles have been studied extensively for their applicability as radiometric standards in the 500-2000 Å region. Under appropriate conditions and with suitable corrections it appears that they can be used reliably in this spectral region having been calibrated with black-body radiation in the visible. A thermopile and a rare gas ionisation chamber have been used to measure independently the same flux at 584 Å and 735 Å, with an agreement better than the estimated reliability of 3 percent. A search is now under way to find a photocathode with a stable photoelectric yield which, in a photodiode, could serve as a convenient and reliable transfer detector standard for the region below 1400 Å. Completed studies prove conclusively that the photoelectric yield of an ultra-clean surface of tungsten can undergo a dramatic change when contaminated by as little as a fraction of a monolayer. That other photocathodes as well are sensitive to contamination is indicated by studies of the effects of ageing and heating on the photoelectric yield of several materials (e.g., gold, chromium) under ordinary vacuum conditions. Anodised aluminium films show promise as surfaces which have a reliable photoelectric yield.

Madden, R. P., **Synchrotron radiation and applications,** Chapter 7 in *X-ray Spectroscopy*, L. Azaroff, Ed., pp. 338-378 (McGraw-Hill Book Co., New York, N.Y., 1974).

Key words: radiation; source and electrons; synchrotron; x-ray, vacuum ultraviolet.

The historical development of the theoretical understanding of synchrotron radiation is reviewed. The important equations necessary to calculate the details of the angular, polarization and wavelength distribution of the radiation and the dependence of these properties on the electron energy and the radius of the trajectory are presented. Also approximate expressions are given which can be utilized to quickly estimate these properties for any given source of synchrotron radiation. The observational development of synchrotron radiation is also historically reviewed, presenting the experimental verification of the theoretical predictions and including a short history of the world's major synchrotron radiation laboratories. Finally, applications of synchrotron radiation in experimental physics are presented, including examples where important contributions have resulted in areas of atomic, molecular, solid state and surface physics as well as in radiometry.

Madden, R. P., **The Frederic Ives Medal for 1971,** *J. Opt. Soc. Amer.* **62,** No. 8, 927-930 (Aug. 1972).

Key words: Ives, medal; medal, Ives; optics, Ives medal.

Ives Medal Citation—Arthur Francis Turner. In recognition of his leadership in pioneering the methods of design and fabrication of multilayer evaporated films; his originality in applying multilayer systems to the solution of practical optical problems; and his effectiveness as an educator, communicating to others the methods and principles he developed during a lifelong devotion to optical physics.

Mahajan, B. M., **Safety standards for home playground equipment,** *Proc. 27th Annual Conf. for Engineering in Medicine and Biology, Philadelphia, Pa., Oct. 6-10, 1974,* **16,** 503 (Alliance for Engineering in Medicine and Biology, Chevy Chase, Md., Oct. 1974).

Key words: component; criteria; development; equipment; hazard; hazardousness; home playground; identification; mishap; misuse; product defect; safety standards; swing set; test method.

Summaries of swing set related accident investigations were examined in order to identify the hazards associated with swing sets. Approximately half of the swing set related mishaps were directly attributed to the design and construction defects of the products. The other half of the recorded mishaps results from improper installation, deterioration or misuse of the product.

Some necessary information, such as anthropometric data, injury threshold data, loading conditions representing child-hazard interactions, and loads applied to certain components to swing sets is presented.

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Quality criteria and test methods are suggested, to establish safety standards for reducing hazards due to design and construction defects of the equipment.

Mahajan, B. M., **Standards for athletic helmets—a state-of-the-art,** *Proc. 27th Annual Conf. for Engineering in Medicine and Biology, Philadelphia, Pa., Oct. 6-10, 1974,* **16,** 181 (Alliance for Engineering in Medicine and Biology, Chevy Chase, Md., Oct. 1974).

Key words: athletic helmets; head injury; injury criteria; safety standards.

The available information on the types of impact induced head injuries, their relative severity, and injury threshold values was collected from the literature. The search revealed that the threshold values are either questionable or are not available.

The literature search revealed that the information regarding the impact conditions which are generated by athletic mishaps is almost non-existent.

A review of standards for helmets revealed that there are no satisfactory performance standards for athletic helmets and that the performance criteria and testing procedures used to evaluate other helmets may be neither appropriate nor adequate for testing athletic helmets.

Mahoney, R., Srinivasan, G. R., Macedo, P. B., Napolitano, A., Simmons, J. H., **Effect of subcritical microstructure on the viscosity of a sodium borosilicate glass,** *Phys. Chem. Glasses* **15,** No. 1, 24-31 (Feb. 1974).

Key words: borosilicate; environmental-relaxation model; glass; microstructure; phase-separation; viscosity.

Viscosity and electron microscopy measurements were made on a phase separating glass as a function of time, at various temperatures. The viscosity changed by five orders of magnitude during the phase separation in a time period identified to be solely in the coarsening stage by electron microscopy. The stage during which composition changes are dominant occurs very quickly despite the high starting viscosity (10^{11} P) and, therefore, is nearly complete before reliable viscosity data can be obtained (2 min). Analysis of the rate of increase of the average particle size identified a rearrangement stage proceeding by bulk diffusion through the fluid phase with an apparent activation energy of 98 kcal/mole (4.1×10^5 J/mole). Superposition of the viscosity-microstructure size curves for various temperatures demonstrated that the change in viscosity was totally controlled by the growth of the viscous phase whose activation energy for viscosity is 132 kcal/mole (5.52×10^5 J/mole). The change of viscosity with time is explained in terms of changes in the size of the microstructure by applying an environmental relaxation model proposed by two of the authors. The significance of the good quantitative fit of the data by the model and the physical significance of the parameters are discussed.

Mandel, J., Steel, M. N., Sharman, L. J., **National Bureau of Standards analysis of the ASTM interlaboratory study of DOC/FF 3-71 flammability of children's sleepwear,** *Amer. Soc. Test. Mater. Stand. News,* pp. 9-13 (May 1973).

Key words: children's sleepwear; flammability; flammability standard; flammability test method.

ASTM Committee D-13 on Textile Materials carried out an interlaboratory study on the test method given in DOC FF 3-71, Standard for the Flammability of Children's Sleepwear. Sixteen laboratories and eight fabrics were involved. D-13's conclusions were that the study demonstrated that laboratories do not obtain the same "pass-fail" results when testing the same fabrics with DOC FF 3-71 as written and, in fact, gross differences in reproducibility were obtained. The same test data was analyzed at NBS. The analysis reported in this paper leads to conclusions contrary to those reported by D-13. The NBS report shows theoretically that with a go-no go test such as that for children's sleepwear, the probability of complete agreement between laboratories is attained only when the material under test is either so far superior to the test method requirements or so far inferior to them that unavoidable test method fluctuations have no effect on the outcome of the test. For a fabric that is only two percent defective, the probability of complete agreement between 16 laboratories is down to 72 percent. The data provide no evidence to support D-13's conclusion that gross differences in reproducibility are obtained.

Martin, W. C., **Low-energy level structure of neutral cerium (Ce I),** *Phys. Rev. A* **3,** No. 6, 1810-1815 (June 1971).

Key words: atomic energy levels; atomic spectra; electron configurations; neutral cerium; Zeeman effect.

The low portion of an extensive level structure derived from analysis of the optical spectrum is reported. Positions, J values, and g_J factors are given for 98 levels, including all 91 levels expected below 10 000 cm^{-1}. A previous report on this analysis showed the ground level to be $4f5d6s^2\ {}^1G_4^\circ$ and gave the lowest levels of $4f5d^26s$. Comparison of the observed odd-parity levels with calculations by Goldschmidt and Salomon shows that all 86 of the odd levels tabulated here belong to these configurations. All but seven of these odd levels are assigned LS names, although the calculations show that many of them have low LS purities, and a few have strong mixtures of the two configurations. The much simpler system of even levels below 10 000 cm^{-1} includes only the six levels of $4f^26s^2\ {}^3H$ and ${}^3F$, beginning with ${}^3H_4$ at 4762.718 cm^{-1} above the ground-state level. The table of even levels also includes $4f^26s^2\ {}^1G_4$ and the lowest two levels of each of the lowest two terms of $4f^25d6s$, ${}^3I_{4,5}$, and ${}^5K_{5,6}$.

Marton, L. L., **Article on Baron Roland von Eötvös,** *Dictionary of Scientific Biography* **4,** 377-381 (1971).

Key words: Eötvös balance; Eötvös' law of surface tension; equivalence of gravitational and inertial mass; geophysical exploration; public service; torsion balance.

Born in 1849 in Badapest, Hungary, he studied in Heidelberg and in Königsberg, Germany. Returning to Hungary he became Professor at the University of Budapest. For a few years he pursued research on surface tension, but after 1888 Eötvös devoted all his research efforts to the problem of gravitation. He designed the "Eötvös torsion balance" and used it for geophysical exploration as well as for measurements of the equivalence of gravitational and inertial mass. He served briefly in the Hungarian Cabinet as Minister of Public Worship and Education, as "Rector" of the University, as President of the Hungarian Academy of Sciences, etc. He died in 1919.

Marzetta, L. A., **A thermesthesiometer—an instrument for burn hazard measurement,** *IEEE Trans. Bio-Med. Eng. BME-21,* No. 5, 425-427 (Sept. 1974).

Key words: burn-hazard; heat-flow; thermal-inertia; thermesthesiometer.

Surface temperature measurement alone is insufficient to establish the hazard to the human of contact with a hot or cold object. A metal surface is more likely to cause thermal injury than a plastic surface at the same temperature. An instrument equipped with a measuring probe has been developed for indicating the temperature that would be experienced if human contact were made with the hot surface in question. The correct value of interface contact temperature can be read for a selected contact time without knowing the composition or temperature of the heated material under test.

McDonald, D. G., Risley, A. S., Cupp, J. D., **The relationship of Josephson junctions to a unified standard of length and time,** (Proc. 13th Int. Conf. on Low Temperature Physics, Boulder, Colo., Aug. 21-25, 1972), Paper in *Low Temperature Physics LT 13,* K. D. Timmerhaus, W. J. O'Sullivan, and E. F. Hammel, Eds., **4,** 542-549 (Plenum Press, New York, N.Y. 1974).

Key words: cryogenics; infrared; Josephson junctions; lasers; superconductivity.

Recent developments have led to large improvements in the frequency stability of infrared lasers. The stability is now comparable with that of the primary frequency standard and greatly exceeds that of the length standard. Thus a stabilized infrared laser could become a unified standard of time (or frequency) and length and replace the two existing standards. A practical problem is that infrared frequency synthesis must be simplified and Josephson junctions show promise for this purpose.

Meese, W. J., **Rules for the operation of electric supply and communication lines and equipment,** Part 4 (Sections 40-43) in the *National Electrical Safety Code,* Sixth Edition, *ANSI C2.4-1973,* pp. 273-313 (IEEE, New York, N.Y., 1973).

Key words: communication industry safety; electrical safety; operation of communication systems; operation of electrical supply systems; public utility safety; safety work rules.

This standard contains Part 4 of the National Electrical Safety Code and supersedes ANSI C2.4-1939, NBS Handbook H34 and pages 305 through 358 of NBS Handbook H30. Part 4 of this Code contains work rules applying to the construction, maintenance, and operation of electric-supply and communication lines and equipment of public utilities and similar systems. These rules are intended to embody the requirements which are most important from the standpoint of safety to employees and to the public.

Meese, W. J., **Safety and safety standards for electric supply and communication facilities in utility tunnels,** *Proc. American Public Works Assoc., Henniker, N.H., Aug. 16-20, 1971, Special Report* **42,** pp. 95-98 (New England College, Henniker, N.H., 1972).

Key words: coordination of utility facilities; national electrical safety code; safety standards for utility tunnels; underground communication facility; underground electric facilities; utility tunnel safety.

In recent years many of the facilities of electric and communication utilities have been installed underground, principally for environmental reasons. Installation and maintenance of these facilities, along with the facilities of several other utilities is becoming difficult and costly, and the necessity of frequent street openings for access to utilities is burdensome to the public and to businesses in the vicinity. Better coordination of utility and other public works facilities is needed. Because of this, the utility tunnel concept is receiving much study and utility tunnel safety is a primary consideration.

Miller, E. F., Jr., Lindamood, G. E., **Structured programming: Top-down approach,** *Datamation* **19,** No. 12, 55-57 (Dec. 1973).

Key words: GOTO statements; hierarchical design; programming; structured programming; top-down design.

Structured programming is the topic of considerable current interest and discussion in computing circles. This informal, tutorial article explains the basic concepts of structured programming—GOTO-less programming, top-down design, and abstract resources—and traces their origins.

Mills, R. M., Yee, K. W., **Walk-through metal detectors for use in weapons detection,** *NILECJ-STD-0601.00,* 26 pages (U.S. Department of Justice, Law Enforcement Assistance Administration, National Institute of Law Enforcement and Criminal Justice, Washington, D.C., June 1974).

Key words: metal detections; performance standards; weapon detection.

A standard has been developed to establish performance requirements and test methods for the detection capability and general characteristics of walk-through metal detectors.

Muehlhause, C. O., **Setting safety standards via risk-benefit analysis,** *Proc. PLP-73 Product Liability Prevention Conf., Newark, N.J., Aug. 22-24, 1973,* pp. 137-140 (1973).

Key words: acceptance of risk; consumer product safety; perception; risk-benefit analysis; standards.

The problem which a hypothetical regulator would face who is intent on setting safety standards for consumer products utilizing the "method" of risk-benefit analysis is examined. It is shown that in addition to a scarcity of difficult-to-produce data certain conceptual problems regarding the manner in which risk to personal health and safety is to be embodied in cost-benefit analysis is also present. A particular formulation which recognizes the acceptance and misperception of risk as well as its cost is presented.

Murphy, T. A., Sengers, J. V., Sengers, J. M. H. L., **Analysis of the pressure of gases near the critical point in terms of a scaled equation of state,** *Proc. Sixth Symp. on Thermophysical Properties, Atlanta, Ga., Aug. 6-8, 1973,* P. E. Liley, Ed., pp. 180-188 (The American Society of Mechanical Engineers, New York, N.Y., 1973).

Key words: carbon dioxide; critical phenomena; critical region of gases; equation of state; parametric equation; scaling laws.

The anomalous thermodynamic behavior of gases near the critical point can be described in terms of scaling laws. In recent years a parametric equation of state, the so-called Linear Model, has been proposed that incorporates the scaling laws. We have developed a method which enables us to determine optimized Linear Model parameters by fitting experimental P-V-T data in the critical region. As an illustration of the method we discuss some preliminary results obtained for CO_2 in the critical region.

Olsen, L., Baumgarten, G. P., **Gas flow measurement by collection time and density in a constant volume,** (Proc. Symp. on Flow—Its Measurement and Control in Science and Industry, Pittsburgh, Pa., May 10-14, 1971), Chapter in *Flow—Its Measurement and Control in Science and Industry,* R. B. Dowdell, Ed., **1,** 1287-1295 (Instrument Society of America, Pittsburgh, Pa., 1971).

Key words: calibration; critical flow; gas flow; measurement; nozzles, volumetric.

A method for the accurate measurement of gas flows is described. This method utilizes a valve to divert the flow to a tank of known volume over a measured calibration time interval. Measurements of pressure and temperature (for gas density) are made when the gas within the tank is at a stationary equilibrium condition. The density increase from essentially zero density within the known volume over the measured time interval permits a determination of the mass rate of flow. The flow measurement apparatus and air treatment system consisting of a centrifugal compressor, air dryer, filters, receiver tank, meter runs, nozzles, diverter valve, collection tank and instrumentation are described. A discussion of the procedures and errors in the measurement of pressures, temperatures, volume of the collection tank and timing of the diverter valve is included. The effects of these individual errors on the overall uncertainty of the gas flow measurement is considered. Ten sonic flow nozzles with throat diameters ranging from 0.14234 to 1.29841 in. were calibrated at upstream pressures to 95 psig and flow rates to 2700 SCFM. On the basis of error analysis and comparisons with calibrations in a bell-type prover, the overall uncertainty of these calibrations is estimated to be about 0.11 percent.

Pilsworth, M. N., Jr., Hoge, H. J., Robinson, H. E., **The thermal conductivity of natural rubber from 134 to 314 K,** *J. Mater.* **7,** No. 4, 580-585 (Dec. 1972).

Key words: glass transition; heat transfer; Hevea rubber; thermal conductivity; thermophysical properties; transport properties.

The thermal conductivity of soft natural rubber, compounded and vulcanized as specified in ASTM recipe 2A, has been measured over a range extending from well below the glass transition to above room temperature. The glass-transition temperature deduced from the thermal-conductivity measurements is 212 K (− 78 F). Most of the measurements were made at the Natick Laboratories in a guarded-hot-plate apparatus, with silicone rubber pads on either side of the sample. The rest of the measurements were made at the National Bureau of Standards with apparatus and procedures that have been used for many years in reference-standard work. The thermal-conductivity data are believed to be accurate to 3 percent or better at room temperature and to about 6 percent at the glass transition and below.

Rabinow, J., **Improving the patent system,** (Proc. Conf. in American Patent Law Association's Annual Meeting, Washington, D.C., Oct. 19, 1972), *American Patent Law Association's Bull.*, pp. 608-625 (Oct.-Nov. 1972).

Key words: antitrust; Department of Justice; human inertia; innovation; inventions; patents and the courts.

The talk touched on the subject of the attacks on the patent system and the recent interest in invention and innovation at the high levels of Government. The relationship between material wealth, the quality of life and the role of the inventor were discussed. The processes of invention and innovation were compared to other games of chance and the effects of adjusting the odds were discussed. A plea was made for raising the odds for the inventor. The talk illustrated the attitude of some members of the Department of Justice and the courts relative to the inventor. The quality of patents as issued by the Patent Office was mentioned, together with a plea to keep the quality as high as possible. The Patent Bar was also asked to improve its ethics and to eliminate the attorneys and some organizations that now are fleecing the unsophisticated inventor. The talk closed with a discussion of the difficulty of introducing an invention into the real world.

Rabinow, J., **Small business R&D—to be or not to be,** *Proc. Conf. II on Survival and Growth: The Small R&D Firm, Sept. 27-29, 1972*, pp. 29-35 (Sept. 1972).

Key words: government contracts; government laboratories; in-house research; patent rights; small company R&D.

The talk concerned small R&D research firms and the difference between those who make a product and those that work strictly as consultants. I discussed the nature of government R&D contracting and the less-than-honorable practices indulged in both by the government and by contractors. The arguments of how much R&D work should be done by government in-house versus outside was touched upon and I pointed out that if the government people are to be competent they must do in-house research and the small R&D firms would do better under such conditions. The question of patent rights was also discussed.

Rabinow, J., **The climate for innovation,** (Proc. First Natl. Conf. Dealing with the Problems of the Small Firms in the Research and Development Industry, Washington, D.C., June 12-14, 1972), Paper in *Survival and Growth. The Small R&D Firm*, J. D. Johnson, Ed., pp. 251-261 (1972).

Key words: consulting services; contract R&D; government contracts; innovation; invention; proposal writing; R&D; small business.

My talk will cover the subject of Small R&D Firms and will be addressed to two types of such firms. One is the small company which develops a product for sale and where R&D is a normal proportion of its business. The other part of the talk will be addressed to R&D companies which do research and development work for industry and Government and whose major effort is not in production.

My talk will criticize both the Government R&D procurement policies and the industry's response. I believe there is considerable inefficiency in the way contract R&D is done, both on the part of the contractor and the contractee.

Renninger, C. R., **Central government structure for the development of an ADP policy,** *Proc. 7th Conf. Intergovernmental Council for ADP, Ottawa, Canada, Sept. 17-19, 1973*, pp. 57-71 (1973).

Key words: ADP policies; computer technology; management; quality control; software.

Advancements in computer technology, the emergence of computer subindustries with new products and marketing strategies, and the growing maturity of both the computer supplier and the computer user are forcing a reexamination of governmental ADP policies. A dominant issue is the management of computer software which has become the critical factor in achieving effective use of computer technology as well as the most expensive element of computer operations. The level of computer effectiveness can be increased significantly by improving software. Better quality control over the production of software is needed to eliminate errors and provide guarantees of satisfactory performance. The utility of proven software needs to be extended to other users to avoid redundant and costly developmental efforts. Ways must be found to reduce the time required to produce software and thereby bring operational systems on-stream sooner. Specific actions taken by the National Bureau of Standards, General Services Administration, and the Office of Management and Budget to improve software management in these areas of need are described.

Richmond, J. C., **Survey of image quality criteria for passive night vision devices,** *LESP-RPT-0301.00*, 22 pages (U.S. Department of Justice, Law Enforcement Assistance Administration, National Institute of Law Enforcement and Criminal Justice, Washington, D.C., June 1974).

Key words: acutance; contrast transfer function; edge gradient; image quality; light equivalent background; light induced background; limiting resolution; line spread function; optical transfer function; point spread function.

Image quality is probably the single most important parameter in determining the utility of any optical device. For night vision devices, in particular, image quality is of paramount importance. In looking at two different photographs of the same scene, which are essentially two different images fixed by the photographic process, almost anyone can tell at a glance which has the better image quality, particularly if there is a significant difference in image quality. Objective evaluation of image quality in quantitative terms is not easy, because there are many variables that contribute to image quality, not all of which have been identified, or can be quantitatively evaluated.

This report is a preliminary survey of image quality evaluation techniques that have been described in the literature and discussion of their merits for use in a standard for passive night vision devices.

Rosenstein, M., Levine, H., McLaughlin, W. L., **A thermosetting radiation-sensing gel for small-volume dosimetry,** (Proc. Fourth Symp. on Microdosimetry, Verbania Pallanza, Italy, Sept. 24-28, 1973), *EURATOM*, J. Booz, H. G. Ebert, R. Eickel, and A. Waker, Eds., pp. 935-950 (Brussels, Belgium, 1974).

Key words: dosimetry; dyes; gels; microdosimetry; plastics; radiochromism; triphenylmethane dyes; vinyl resins; x-ray detectors.

Thin-film radiation detection systems using triphenylmethane dye derivatives have been developed previously, and their dosimetric properties have been described in the literature. Until the present work, the solid activator matrix that best sensitized radiolytic dye production was gelatin. Gelatin has the serious problems of dimensional instability and migration of the dye formed after irradiation. The im-

proved activator matrix described here has potential wide application as a radiation detector and imaging system. The dosimeter response results from conversion of the dye precursor to the colored dye, and is a nearly linear function of absorbed dose. Due to the nonturbid matrix, image resolution of 1 μm can be achieved using microdensitometry.

The most successful formulation of those investigated to date contains: a triphenylmethane dye precursor; a specific combination of monomers and polymers, which constitute the activator matrix; and a polymerization initiator. The thermosetting formulation can be molded into a solid glassy resin. Its elemental constituents are C, H, N, and O, and its mass energy absorption coefficient for photons above 200 keV is within 4 percent of that for water and muscle. Down to at least 25 keV, there is no significant variation of dosimeter response with photon energy. Variation of response with ambient temperature during irradiation of the system, relative to room temperature, is less than ± 5 percent between 0-50 °C. After irradiation and a slight initial 24-hour color buildup, the image is stable for about 1 month. Then a gradual fading occurs. With a 2 mm-thick gel, absorbed doses of 10 krad can be detected with precision limits of 5 percent.

Ross, P. D., Goldberg, R. N., **A scanning microcalorimeter for thermally induced transitions in solution,** *Thermochimica Acta* **10,** 143-151 (1974).

Key words: biopolymer transitions; calorimetry; chemical instrumention; dipalmitoyl L-α-lecithin; microcalorimeter; thermochemistry.

A scanning microcalorimeter for the measurement of energies of transition in solution is described. The calorimeter utilizes semi-conductor thermoelectric modules and is of a very simple and inexpensive construction. The imprecision of measurement is three percent when measuring 25 to 250 mJ of heat associated with transitions over temperature intervals of up to 8 K. The calorimeter operates from ambient to 90 °C.

Ruegg, F. W., Johnson, D. P., **Dynamics of the bell prover,** (Proc. Symp. on Flow—Its Measurement and Control in Science and Industry, Pittsburgh, Pa., May 10-14, 1971), Chapter in *Flow—Its Measurement and Control in Science and Industry,* R. B. Dowdell, Ed., **I,** 1297-1307 (Instrument Society of America, Pittsburgh, Pa., 1971).

Key words: bell prover; dynamics of provers; flow measurement; gas flow measurement; prover design.

The bell prover is widely used for gas flowrate measurement by timing a known stroke of the bell as it rises, with presumably constant speed, from a bath of sealing liquid. A motion analysis of the coupled fluid and mechanical parts of the prover system has been made to guide experiments, and to determine dynamic use criteria and measurement errors associated with transient oscillatory motions. Simultaneous differential equations for the motions of the bell, sealing liquid, and gas are presented as a basis for a computer simulation of prover performance. Motion of the bell is considered as affected by the gas pressure therein, by the masses in motion, by viscous drag force and adherence of liquid. Pressure and gravity forces, and viscous flow resistance, affect the liquid motion. Gas pressure in the bell is affected by all the motions and by the gas content. Various methods of damping initial transient motions are included in the analysis.

Rupp, N. W., **Clinical use of some dental materials. Part I. Amalgam,** *J. Indiana Dent. Assoc.,* pp. 432-434 (Oct. 1973); **Part II. Composite restorative materials,** 491-495 (Nov. 1973).

Key words: acid etch; burnishing; handling techniques; materials; restorative.

This discussion of selected dental restorative materials covers new developments in both materials and handling techniques. Dental amalgam alloy formulations and the burnishing of restorations at the time of placement are included. Luting agents, esthetic restorations and acid etch enhanced retention are also covered for the information of the practicing dentist. The review has 34 references.

Rush, J. J., Livingston, R. C., Rosasco, G. J., **Raman scattering study of crystal dynamics and order—disorder transitions in alkali hydrosulfides,** *Solid State Commun.* **13,** 159-162 (1973).

Key words: alkali hydrosulfides; crystal dynamics; Raman scattering.

Raman spectra have been measured for NaSH, CsSH and RbSH over a range of temperatures from 85 to 400 K. The results show that the order—disorder phase transitions in these solids are associated with significant changes in the details of their crystal dynamics. In addition the Raman spectra provide clear evidence for the existence of previously unobserved low-temperature phases in each compound, which apparently involve total ordering of the SH^- ions.

Rush, J. J., **Study of large-amplitude vibrations in molecules by inelastic neutron scattering,** (Proc. Conf. Critical Evaluation of Chemical and Physical Structural Information, Dartmouth College, Hanover, N.H., June 24-29, 1973), Paper in *Critical Evaluation of Chemical and Physical Structural Information,* D. R. Lide, Jr., and M. A. Paul, Eds., pp. 369-385 (National Academy of Sciences, Washington, D.C., 1974).

Key words: barriers to rotation; large amplitude vibrations; momentum transfer; neutron scattering; optical spectroscopy; torsional vibration.

The application of neutron inelastic scattering to the study of large amplitude intramolecular (primarily torsional) vibrations in hydrogeneous molecules is discussed. In principle the neutron technique provides an excellent complement to optical techniques, due in part to the fact that large-amplitude modes, which are sometimes inactive or weakly active in IR or Raman spectra, provide intense peaks in neutron spectra. However, relatively poor ($\sim 10\ cm^{-1}$) instrumental resolution and Doppler broadening effects in fluid phases sometimes cause significant complications in experiment and interpretation. Neutron spectral results on several prototype methyl-substituted molecules are presented and compared with relevent optical data. Some of the limitations and pitfalls of neutron molecular spectroscopy are discussed along with the difficulties in deriving potential barrier parameters from a limited number of torsional mode assignments.

Saltman, R. G., **Educating public administrators for managing science and technology,** *Pub. Admin. Rev.* **34,** No. 4, 394-396 (July-Aug. 1974).

Key words: administration; education; information; management; public; science; technology transfer.

Public administrators are being forced to increasingly consider science and technology in decisions that they make concerning both plans and operations. In order to manage and control pertinent science and technology and to effectively employ them, the public administrator needs a professional education which gears him for these tasks. Information science and management science are applications-independent tools that the administrator can use extensively to make his operations more efficient, to provide him with the coordinated information he needs, and to provide him with a rational, analytic basis for decision-making about the utilization of all forms of science and technology. At present, there is no recommended or generally accepted curriculum for educating public administrators for managing science and technology. The academic community in Public Administration, with assistance from the information science

and management science communities, should form a committee to recommend a curriculum in this area.

Schaffer, R., **Diagnostic materials for clinical analysis,** (Proc. Int. Conf. on Standardization of Diagnostic Materials, Atlanta, Ga., June 5-8, 1973), Paper 1 in *Bull. Wld. Hlth. Org.* **48,** 715-720 (1973).

Key words: clinical chemistry; clinical standards; diagnostic kits; diagnostic material; standard reference materials for clinical chemistry; standards.

Standardization of diagnostic materials has lagged behind their development and application. The need to improve the accuracy of the results obtained with them has stimulated collaborative efforts to upgrade the quality of the reagents, control materials, and standards used, with the result that specifications for reagents and standards and authoritative standard materials are now available for a number of clinical tests. Achievements thus far and the efforts now in progress are reviewed.

Scott, W. W., Jr., **A new coaxial RF-DC ammeter, (Summary),** (Proc. Conf. Digest on Precision Electromagnetic Measurements, Boulder, Colo., June 2-5, 1970), Special Issue *CPEM Digest,* p. 13 (1970).

Key words: ammeter; compensation; radio-frequency; RF-DC difference; standard; thermal-current-convertor; thermopile.

A small, portable reference standard of radio-frequency current has been developed which, when calibrated with the NBS Standard Electrodynamometer, will serve as an interlaboratory standard of high accuracy between NBS and users in industry.

The ammeter is unique and has no precedence in principle of operation. It consists of an elliptic cylindrical silver reflector of infrared energy with a cylindrical thin-film quartz heater along one focus and a heat sensing thermopile along the other focus.

The ammeter has three times the current range of older ammmeters with up to ten times larger output and unequalled broadband frequency range. The prototype covers 0.5 ampere to 5 amperes (heater burnout at about 9 amperes) with corresponding dc outputs from 1 millivolt to 100 millivolts for currents in the frequency range dc to 1 GHz.

Sengers, J. M. H. L., **Critical point,** *Encyclopedia Americana* **8,** 219-220 (Americana Corp., New York, N.Y., 1973).

Key words: critical anomalies; critical opalescence; critical point; critical-point phase transitions.

For the general reader, the critical point is defined using the gas-liquid system as an example. Critical anomalies and light-scattering methods for studying these are discussed. Some further examples of critical-point phase transitions are enumerated and their analogy is stressed.

Siegwarth, J. D., Radebaugh, R., **The Kapitza resistance between Cu(Cr) and ^{4}He(^{3}He) solutions and applications to heat exchangers,** (Proc. 13th Int. Conf. on Low Temperature Physics, Boulder, Colo., Aug. 21-25, 1972), Paper in *Low Temperature Physics LT 13,* K. D. Timmerhaus, W. J. O'Sullivan, and E. F. Hammel, Eds., **1,** 398-400 (Plenum Press, New York, N.Y., 1974).

Key words: alloy; copper; dilution refrigerator; Kapitza resistance.

The Kapitza resistance of work hardened copper has been found to be as much as ten times lower than that of annealed copper below 0.1 K. There are other hardening techniques which can be used for copper, such as oxygen annealing of copper containing small amounts of such impurities as Al, Be or Si or precipitation hardening of copper containing small amounts of Cr or Zr. We have measured the Kapitza resistance between a precipitation hardened alloy of Cu – 0.6 atomic percent Cr and the dilute He^3 stream in a dilution refrigerator. With the proper heat treatment, Cu(Cr) has a Kapitza resistance ten times smaller than annealed OFHC copper. The thermal conductivity of Cu(Cr) is about 0.1 that of OFHC copper. This is sufficient for use in heat exchangers in dilution refrigerators. Such an exchanger may be fabricated by sintering in H_2 at ~ 750 °C, then heat treating at ~ 450 °C to obtain low Kapitza resistances.

Simiu, E., **Improved methods for determining wind profiles and dynamic structural response to wind,** *Proc. ASCE-IABSE Regional Conf. on Tall Buildings, Bangkok, Thailand, Jan. 1974,* pp. 491-503 (1974).

Key words: aerodynamics; dynamic response; gust factor; structural engineering; wind profiles; wind spectra.

In current methods for determining alongwind structural response, it is assumed that wind profiles are described by empirical power laws and that turbulence spectra are independent of height. In this paper, the adequacy of these assumptions is assessed in the light of recently established results of boundary layer meteorology. An improved method for determining wind profiles is presented, and expressions for the dynamic alongwind response, including deflections and accelerations, are proposed. In addition to the variation of wind spectra with height, these expressions take into account the pressure correlations in the alongwind direction, determined in accordance with basic theory and known experimental results.

Simiu, E., **Variation of mean winds with height in hurricanes,** *J. Eng. Mech. Div. Am. Soc. Civil Eng. Tech. Note* **100,** No. EM4, 833-837 (Aug. 1974).

Key words: boundary layer; hurricanes; loads (forces); natural disasters; structural analysis; tall buildings; wind profiles.

The magnitude of wind pressures on buildings and structures depends, among other factors, upon the variation of wind speeds with height. The presence in hurricane flows of strong inertial forces due to the curvature of the isobars in the region of highest winds suggests that differences exist between hurricane velocity profiles and the logarithmic profiles typical of extratropical winds. Simplified models of boundary layer flow in cyclostrophic and geostrophic flow are used to show that these differences appear to be significant. The results obtained suggest that an investigation based on a more realistic model of actual atmospheric boundary layer flow is warranted. Suggestions are made for the major ingredients of an alternative model and the use of existing models for numerical solution of the model. These indicate the feasibility of getting more reliable estimates for the variation of the winds with height under hurricane conditions. The author is currently conducting research along the lines indicated.

Snell, J. E., Achenbach, P. R., **Total energy systems: A review of recent NBS activities,** *Proc. Effective Energy Utilization Symp., Drexel University, Philadelphia, Pa., June 8-9, 1972,* pp. 201-233 (June 1972).

Key words: central utility systems; electrical power generation; energy conservation; energy costs; integrated utility systems; total energy systems, waste disposal.

This paper briefly reviews and reports on the status of several NBS activities in the area of total energy systems as they relate to the theme of the Drexel Symposium on Effective Energy Utilization. A recent review of the state of the art in total energy systems application, indicated the need for good, concise, operating and performance data on total energy systems to serve as a basis for more effective utilization of this concept to save energy. The Department of Housing and Urban Development requested NBS to assist in the development of a total energy system on the BREAKTHROUGH housing site at Jersey City and to conduct a full-scale field study with appropriate instrumentation to obtain engineering, cost and maintenance data.

In a related effort, NBS, AEC, EPA, and NASA are supporting HUD in a new effort entitled The Modular-Sized Integrated Utility

System (MIUS) program. The premise of this 3-phase effort is to demonstrate the potential energy, resource, and cost economies of combining energy-generating facilities and waste disposal facilities on a modular-basis to keep pace with changing patterns and rates of urban growth.

Somes, N. F., Corley, W. G., **Circular openings in webs of continuous beams,** *Amer. Concrete Inst. Spec. Publ. 42-17*, pp. 359-398 (1973).

Key words: beams; design criteria; joists; openings; shear strength; tests; web.

The second phase of a comprehensive investigation is reported. Tests show the effect on strength and behavior of circular web openings in continuous lightweight-aggregate concrete joist floors. Principal variables were size, location, reinforcement and spacing of openings. Based on the findings, design recommendations are presented.

Somes, N. F., **Experience with the development and application of structural performance criteria,** (Proc. Workshop on Systems Building, NBS, Gaithersburg, Md., Feb. 24-26, 1972), Paper in *Systems Building*, pp. 269-292 (Available from the National Technical Information Service, Springfield, Va. 22161, 1972).

Key words: building; evaluation; performance criteria; physical simulation; structural safety; structural serviceability.

The paper is based upon experience gained by the author as a member of the NBS team which over the past two years has served as the technical arm of HUD in Operation BREAKTHROUGH. A brief introduction to the nature of BREAKTHROUGH is followed by a description of the task of preparing the Guide Criteria. The housing system producers within the program were required to submit evaluation documents. These are described together with the experience of the evaluation team in dealing with these documents. Recommendations are given as to the ways in which future evaluations might avoid difficulties and time delays. When it is not possible to evaluate through this submission of documents it may be necessary to use physical simulation. To illustrate this technique a case history is presented of the evaluation of the system which used concrete box modules.

Soulen, R. J., Jr., Marshak, H., **The use of Josephson junctions for noise thermometry below 1 kelvin,** *Proc. Applied Superconductivity Conf., Annapolis, Md., May 1-3, 1972*, pp. 588-591 (1972).

Key words: beryllium; Co^{60} γ-ray anisotropy thermometer; Josephson junction; low temperature thermometry; noise thermometry; superconductivity.

Kamper and Zimmerman have demonstrated that a Josephson junction connected in parallel to a resistor converts the Johnson noise voltage fluctuations into frequency fluctuations, and that the variance of these frequency fluctuations is simply related to absolute temperature. In order to make accurate measurements of temperature with this device, a fast data acquisition system consisting of a frequency counter interfaced to a small computer has been developed. This thermometer has been compated to a Co^{60} γ-ray anisotropy thermometer in the temperature region of .020 to .050 K. Preliminary results indicate agreement to within 5 percent. We have used our results to redetermine the superconductive transition temperature of pure beryllium. Our value is .0228 K, 3mK lower than reported by Falge. Since our thermometers do not depend upon any calibration or extrapolation and only on some accurately and independently determined parameters of each system, our value of T_c is probably very close to the *absolute* temperature of the transition.

Steiner, B., **New needs for accurate optical radiation measurements. II. A growing concern of the National Bureau of Standards and of American CIE,** *Proc. Conf. on Photometry and Colorimetry, Varna, Bulgaria, June 27-30, 1973*, pp. 39-45 (Dec. 1973).

Key words: energy crisis; health; meteorology; photometry; pollution monitoring; radiometry; remote sensing; safety.

Moreover, commercial needs and concern for more accurate optical radiation measurement are paralleled by growing public problems whose solutions depend strongly upon improved radiometry and photometry. The recent rapid growth of the electro-optics industry has both caused and exacerbated the severity of the measurement difficulties. The resulting great technical effort required can be justified by the public issues involved as well as by the commercial impact. Examples of these public issues are: the health issues of phototherapy and clinical analysis; the safety issues of potential destruction of the protective earth ozone layer, biomedical engineering, and transportation; the energy crisis; meteorology; pollution monitoring; and remote sensing. The effort to achieve a larger and more coordinated approach to the related radiometric and photometric problems have been organized by American CIE TC 1.2 through its creation of the Council for Optical Radiation Measurement. The purpose, structure, and activity of the Council are described.

Stillman, R. B., **A survey of techniques for increasing software reliability,** *Proc. Summer Computer Simulation Conf., Montreal, Canada, July 1973*, pp. 1130-1133 (1973).

Key words: dynamic analysis; proof of correctness; software reliability; static analysis; testing software.

The quality of today's major software systems is uneven at best. Programs thought to be correct will suddenly produce wrong results, no results, or behave otherwise erratically, because some special condition in the data or in the environment was not accounted for in the logic of the program. Techniques to improve reliability and to facilitate thorough testing of software fall into two main categories: (1) Static analysis, which is performed without executing the software. Questions of overall software system design, higher-level language design, use of various static analysis tools, and the concept and potential of machine generated proofs of correctness are addressed; (2) Dynamic analysis, which is dependent upon information collected while the software is in execution. Interest is centered on frequency (of execution) monitors; dynamic debugging facilities, address range and data bound checks, optionally compilable assertions, and tracing and tracking tools.

Sugar, G. R., **Voice privacy equipment for law enforcement communication systems,** *LESP-RPT-0204.00*, 27 pages (U.S. Department of Justice, Law Enforcement Assistance Administration, National Institute of Law Enforcement and Criminal Justice, Washington, D.C., May 1974).

Key words: intelligibility; LESL; NILECJ; performance standard; privacy; scramblers; speech quality; speech scramblers; survey; testing; voice privacy.

Law enforcement agencies are finding an increasing need for voice-scrambling equipment to provide privacy on their two-way radio communication systems. Work is underway at the National Bureau of Standards, under the sponsorship of the National Institute of Law Enforcement and Criminal Justice (NILECJ), to develop performance standards for voice scramblers. The four areas being considered are speech intelligibility, voice quality, voice privacy, and general system characteristics. This report first defines a set of special terms, then describes a number of types of scramblers that are now available for law enforcement use. Some inherent problems and weaknesses are discussed. The concepts of intelligibility and privacy are explored in detail. The potential contents of the standard are described, and some problems inherent in preparing and using the standard are discussed. The report concludes with some material intended to be of immediate assistance to the prospective purchaser of scramblers: a survey of units now on the market, some hints on how

to proceed in the absence of a standard, and a bibliography of technical publications on voice scrambling.

Suzuki, G., Hendrickson, R., Donaldson, J., **Quantitative methods in decisionmaking,** Chapter VI in *Management: Concepts and Practice*, F. R. Brown, Ed., pp. 115-155 (Industrial College of the Armed Forces, Ft. McNair, Washington, D.C., 1972).

Key words: decisionmaking; methods; models.

This paper is a revision of Chapter VIII of a handbook used by the Industrial College of the Armed Forces. The handbook has the full title *National Security Management-Management: Concepts and Practice*, and is required reading for students attending the College. Chapter VIII is one of three chapters of Part II of the book dealing with the general subject *Quantitative Tools for Management*. The intent of the chapter is to introduce the reader, who is assumed to have no knowledge of the subject, to the principal elements and kinds of decision processes that occur in operations that require explication and analysis. The chapter is divided into nine sections, whose organization and content lead the reader through an ordered development of the material, dealing with the qualitative and quantitative aspects of the problems likely to be faced and the practicable methods used in the formulations and solutions of these problems. Optimizing and non-optimizing analyses are covered appropriately for the needs of the intended audience of the book. The authors have tried to state the limited utility of formal mathematical methods and have apprized the reader of the fundamentals of operations research as they contribute to problem-solving and analysis of operational situations.

Swanson, N., Celotta, R. J., Kuyatt, C. E., **Resonant structure in electron impact excitation of xenon,** (Proc. VIII Int. Conf. on the Physics of Electronic and Atomic Collisions, Beograd, Yugoslavia, July 16-19, 1973), Abstracts of Papers of the *VIII International Conference on the Physics of Electronic and Atomic Collisions*, B. C. Cobic and M. V. Kurepa, Eds., **I,** 478-479 (Institute of Physics, Beograd, Yugoslavia, May 1973).

Key words: electron impact; uv lasers; xenon excitation functions.

Electron impact excitation functions for atomic xenon are presented.

Tate, E. L., **On the interlibrary loan horizon—non-mechanical,** *Proc. First Annual Federal Interagency Field Librarians Workshop, Washington, D.C., Sept. 24-28, 1972*, pp. 277-282 (1972).

Key words: federal libraries; interlibrary loans.

The paper describes two studies on interlibrary loans sponsored by the Association of Research Libraries. One, published this spring, concerns the characteristics, costs, and magnitude of interlibrary loans in academic libraries; the other, being prepared under contract from the National Commission on Libraries and Information Science, will deal with the feasibility of centralized or regionalized interlibrary loan centers. Comments on the current state of the copyright/photocopying problem are included. Present and proposed projects of the Federal Library Committee Task Force on Interlibrary Loan Arrangements are discussed.

Taylor, B. N., **Cryogenic metrology,** (Proc. 13th Int. Conf. on Low Temperature Physics, Boulder, Colo., Aug. 21-25, 1972), Paper in *Low Temperature Physics LT 13*, **4,** 465-482 (Plenum Press, New York, N.Y., 1974).

Key words: cryogenics; fundamental constants; instrumentation; metrology.

The application of cryogenic technology and phenomena to selected areas of metrology is discussed. While the several and varied uses of the Josephson effects in the solution of metrological problems is the main topic reviewed, some past and present metrological uses of non-Josephson related low temperature phenomena are included. Prognostications regarding the future of the field are also given.

Taylor, J. K., Zielinski, W. L., Jr., Maienthal, E. J., Durst, R. A., Burke, R. W., **Development of method for NTA analysis in raw water,** *U.S. Environmental Protection Agency EPA Report R2-72-057*, 34 pages (Sept. 1972).

Key words: chemical analysis; nitriolotriacetic acid; NTA; water analysis; water pollution.

The free acid form of nitrilotriacetic acid is readily esterified by N,O-bis(trimethylsilyl)acetamide and gas chromatographic analysis is directly applicable to this derivative. The response characteristic of NTA-trisilylester was 2,200 mm^2 peak area per microgram of NTA at maximum sensitivity of the hydrogen flame ionization detector. Accordingly, gas chromatography has the potential for detecting NTA concentrations of practical interest providing that suitable NTA isolation techniques can be developed.

The cupric ion-selective electrode provides the basis for a sensitive electrochemical detector for NTA. Apparatus for the on-stream determination of uncomplexed NTA has been developed. This may be used for determination of total NTA, after the latter is separated from bound metal ions and other complexing agents by a suitable means, such as ion-exchange chromatography.

Polarographic studies have shown that the bismuth-NTA complex is a suitable method for the determination of NTA in most waters. While some metal ions may interfere, a pre-electrolysis step and/or a standard addition technique seems feasible to eliminate this problem.

Potentiometric titration with cupric ion should provide a rapid and reliable referee method for the determination of NTA in detergent formulations. Such a method would appear to be superior to the spectrophotometric methods presently used, since the latter are affected by turbidities which are encountered in many of the samples.

Thomas, D. B., Freeze, P. D., **The effects of catalysis in measuring the temperature of incompletely-burned gases with noble-metal thermocouples,** *Proc. 5th Symp. Temperature—Its Measurement and Control in Science, Washington, D.C., June 21-24, 1971*, pp. 1671-1676 (1971).

Key words: butane; carbon monoxide; catalysis; combustion; hydrogen; optical pyrometer; platinum; platinum-13 percent rhodium; temperature; thermocouple.

Measurements have been made on the effects of catalysis when platinum-13 percent rhodium versus platinum thermocouples are used to measure the temperature of incompletely-burned gases in the temperature range 1000 to 1500 °C. These measurements indicate that significant temperature errors can result when noble-metal thermocouple materials are exposed to various unburned gases under laboratory test conditions. Platinum and platinum-13 percent rhodium thermocouple elements were exposed to gas mixtures of air + 1.0 percent H_2, air + 2.0 percent H_2, air + 1.0 percent CO + 0.01 percent H_2, air + 2.0 percent CO + 0.01 percent H_2 and air + 0.5 percent C_4H_{10}. At very low gas velocities ($< 9 \times 10^{-3}$ m/second), the thermoelement temperature increase due to surface combustion varied from about 2 to 77 °C at thermoelement temperatures between 1000 and 1500 °C. At gas velocities between 0.17×10^2 and 1.83×10^2 m/second, the temperature increases varied between 35 and 380 °C. Measurements with five gas mixtures indicate that the sample temperature increases (ΔT) due to catalytic heating increase with increasing gas velocity up to approximately 1.2×10^2 m/second. Above 1.2×10^2 m/second, the ΔT values tend to decrease with further increasing velocity.

Thurber, W. R., Bullis, W. M., **Resistivity and carrier lifetime in gold-doped silicon,** *Air Force Cambridge Research Laboratories*

Report AFCRL-72-0076, 37 pages (Air Force Cambridge Research Laboratories, Air Force Systems Command, U.S. Air Force, Bedford, Mass. 01730, Jan. 31, 1972).

Key words: carrier lifetime; gallium arsenide; gold-doped silicon; resistivity; silicon; surface photovoltage.

This report describes the present status of an on-going study of the properties of gold-doped silicon. Resistivity, Hall effect, and carrier lifetime are being measured at room temperature in silicon wafers doped with varying amounts of gold and either phosphorus or boron. Reasons are being sought for the apparent discrepancy between total and electrically active gold, for the discrepancy between calculated and observed resistivity in both *n*-type and *p*-type specimens with very large gold concentration, and for the diversity in capture cross-section data reported in the literature. Although many questions still remain, progress has been made in resolving these discrepancies. There is considerable evidence that the low resistivity observed at large gold concentrations is associated with the introduction of shallow acceptor states in concentrations strongly dependent on the gold concentration. The origin of these states is being sought. Initial studies of the application of the surface photovoltage method to the measurement of carrier lifetime in gold-doped silicon have been completed. This method also appears to be suitable for use on gallium arsenide specimens. A bibliography of the literature on properties of gold-doped silicon that contains 136 entries is also included as an appendix.

Trechsel, H. R., **Structural performance testing of windows, curtain walls, and doors,** *Amer. Soc. Test. Mater. ASTM Spec. Tech. Publ.* **552,** pp. 36-41 (1974).

Key words: curtain walls; doors; test; walls; wind loads; windows.

This paper is a commentary on the ASTM Test for Structural Performance of Exterior Windows, Curtain Walls, and Doors under the Influence of Wind Loads, Designation E 330-70. A brief historical background of the development of the test method is given, the procedure is summarized, some of its features are highlighted, and the use, application, and significance of the method are discussed.

Utech, H. P., **Status report on research programs for firefighters protective clothing,** *Proc. Fire Department Instructors' Conf., Kansas City, Mo., Mar. 27-30, 1973,* pp. 156-166 (1973).

Key words: comfort; fire coat; firefighting; impact protection; injury statistics; protective clothing; thermal conditions; turnout coat.

The inadequate design of present-day protective clothing and equipment used by firefighters can be attributed to a lack of quantitative data on what that equipment is expected to do and underwhat conditions it must perform. Research on firefighters' turnout gear at the National Bureau of Standards has focused on developing the needed quantitative data. Progress in defining the hazards faced by firefighters, measuring the performance of present-day coats, quantifying the thermal conditions to which firefighters are exposed, predicting the performance of protective equipment under those conditions, and using this information to specify the design of improved turnout gear is described.

Vadelund, E. A., **Change to metric can maximize package size rationalization,** *Proc. DFISA Conf., Las Vegas, Nev., Mar. 28, 1973,* pp. 45-48 (1973).

Key words: labeling; metric system; packaging; size rationalization; state and federal laws and regulations.

Presents a brief overview of the current status of metrication including legislative activities. Outlines the changes that need to be considered by the packaging industry in the event a measurement system change occurs.

Velapoldi, R. A., Diamondstone, B. I., Burke, R. W., **Spectral interpretation and kinetic studies of the $Fe^{3+} - H_2SO_4$ (Zak) procedure for determination of cholesterol,** *Clin. Chem.* **20,** No. 7, 802-811 (1974).

Key words: carbonium ions; cholesterol; enylic ions; isosbestic points; kinetics; reaction mechanisms; steroids; Zak procedure.

Spectral changes and kinetic data presented for the Zak reaction show the pseudo-first-order character of the consecutive oxidative reactions undergone by cholesterol and selected steroid dienes. These data give excellent support to the proposed formation of the homologous series of steroidal enylic cations which are the absorbing species in the spectrophotometric cholesterol determination. Typical thermodynamic quantities of ΔG_+, ΔH_+, ΔS_+ and E_a are also reported for several different reactions. Low acetic-sulfuric acid ratios evidently result in the stabilization of the lower members of the homologous enylic series. Although excellent reproducibilities are obtained for premixed and non-premixed Zak reagents, it is necessary to use the premixed reagent if good temperature control is required, as would be the case for kinetic methods of analysis run under the conditions we used. The isosbestic point observed at 503 nm may also be used as an analytical wavelength because it is less sensitive to variables such as temperature, time, and steroid concentration. (+ symbolizes that the letter to which it is superscript is a thermodynamic parameter for the activated complex and not for the overall reaction.)

Velapoldi, R. A., Wicks, S. A., **The use of chemical spot tests kits for the presumptive identification of narcotics and drugs of abuse,** *J. Forensic Sci.* **19,** No. 3, 636-656 (1974).

Key words: centroid color charts; color spot tests; drugs of abuse; experimental detection limits; field tests; narcotic identification; narcotics; spot tests; street drugs.

Numbers and colors from the Inter Society Color Council—National Bureau of Standards Centroid Color Charts have been assigned to the colors produced by the reactions of typical narcotic field test reagents with pure drugs and other substances. A short discussion of the colors produced with street samples of drugs is also given. Flow charts are presented whereby increased selectivity is obtained by multiple reagent testing. Experimental detection limits were obtained for two drugs, heroin and LSD, by a rigorous, statistically meaningful method and for several other drugs by a less rigorous method. Reagent stabilities and temperature effects are also discussed. It is evident that narcotic field test kits can be useful in obtaining presumptive or preliminary information.

Waksman, D., Ferguson, J. B., **Fire tests of building interior covering systems,** *Fire Technol.* **10,** No. 3, 211-220 (Aug. 1974).

Key words: Fire hazard properties; gaseous combustion products; interior covering systems; interior finishes; smoke generation; surface flammability.

The fire performance of assemblies consisting of surface coverings applied over two types of painted substrates was investigated. Relatively noncombustible asbestos cement board (ACB) and painted plywood intended to represent a combustible substrate were used. Properties measured included surface flammability, and smoke density and gaseous combustion product levels. Considerable substrate dependence was found for these properties. On the basis of the results observed in this study, it is concluded that it would be advantageous to base fire safety ratings on the results of tests conducted on coverings applied to both combustible and noncombustible substrates.

Walker, J. C., Hughes, C. E., **POPSS—a parametric operating system simulator,** *Proc. SIGCSE Meeting, Columbus, Ohio,* pp. 166-169 (1973).

Key words: computer system; FORTRAN IV; operating system; resource allocation strategies; simulator.

In this paper we describe POPSS, an event driven simulator which is intended to simulate the activity of a computer system—hardware together with an operating system—as it processes a workload. Input to the simulator is in the form of keyword parameters which are used for describing all three components—hardware, operating system, and workload.

POPSS is a simulator as opposed to a simulation language. It is designed to model the inner workings of a computer system in addition to yielding the results usually associated with simulation. The program is highly modular, consisting of some 45 subprograms. Of these, there are 22 modules, each of which represents an operating system component (or possibly a part of one such component). Included in POPSS are built-in replacement features to allow a user the capability of designing alternative resource allocation strategies. These features are in addition to the standard subprogram replacement automatically available through the use of FORTRAN IV.

Wall, L. A., Roestamsjah, Alridge, M. H., **Pyrolysis of mixtures of monodisperse poly α-methylstyrenes,** *Amer. Chem. Soc. Polymer Preprints* **13,** No. 2, 1041-1043 (Aug. 1972).

Key words: polymers; pyrolysis; poly α-methylstyrene, zip-length.

Mixtures of monodisperse poly α-methylstyrenes were pyrolyzed and their rate of weight lost measured as a function of molecular weight. The pyrolytic weight lost of poly αtrideuteromethyl β, β dideuterostyrenes were also studied. This polymer gives pure monomer as a volatile product and has a large zip-length. For very large zip-length compared to molecular weight, theory predicts a rate proportional to weight average degree of polymerization. We observed a dependence in excess of the weight average D, P. in the region that the rate is approximately proportional to molecular weight. This is suggestive of an effect related to the physical properties of the liquid melt in the direction to increase the zip-length.

The present results on monodisperse polymers indicate longer zip-lengths than previously estimated from measurement on fractionated poly α-methylstyrenes. Also the monodisperse deuterated polymers have an even longer zip-length compared to the nondeuterated polymers.

Wall, L. A., **Condensed phase combustion chemistry,** *Fire Res. Abstr. Rev.* **13,** 204-219 (1971).

Key words: burning of polymers; combustion; ignition; polymer decomposition; pyrolytic decomposition.

The role of the chemical pyrolytic decomposition mechanisms of polymer decomposition in the ignition, combustion and burning of polymers is outlined in the light of available information. The particular aspects discussed are: mechanism, effect of conditions, catalytic effects, energetics, types of decompositions induced and oxidative degradation, burning of polymers, heats of gasification and regression rates.

Warkulwiz, V. P., Mozer, B., Green, M. S., **Observation of the deviation from Ornstein-Zernike theory in the critical scattering of neutrons from neon,** *Phys. Rev. Lett.* **32,** No. 25, 1410-1413 (June 24, 1974).

Key words: critical exponent η; critical point; critical scattering; neon; neutron diffraction; Ornstein-Zernike.

A deviation from the Ornstein-Zernike theory of critical scattering has been observed in a neutron-diffraction study of neon near its critical point. The critical exponent η was determined to have the value $0.11^{+0.03}_{-0.02}$.

Walter, L. S., French, B. M., Heinrich, K. F. J., Lowman, P. D., Jr., Doan, A. S., Adler, I., **Mineralogical studies of Apollo 12 samples,** (Proc. Second Lunar Science Conf. Houston, Tex., Jan. 11-14, 1971), *Geochim. Cosmochim. Acta Suppl. 2,* **1,** 343-358 (1971).

Key words: Apollo 12; crystallization; mineralogy; moon; petrography; pyroxene; rocks.

The five crystalline rocks studied represent three distinct chemical groups: (1) low-Mg, high-Al; (2) intermediate; and (3) low-Al, high-Mg. Petrography and mineral compositions are consistent with the suggestion that the differences reflect olivine removal during crystallization, producing Mg-rich cumulate rocks and Mg-poor residual liquids. Some mineralogical characteristics are consistent with this model. However, significant mineralogical differences are observed between specimens in the same chemical group, suggesting that the actual crystallization relations are more complex. Ni-Fe metal, possibly emplaced as a late-stage vapor deposit, occurs in cracks in pyroxene and chromite, and along pyroxene cleavage elements. The metal has the same nickel content as other metal in the sample and is not associated with sulfide. No concentration gradients in iron in the host crystal are observed.

Waterstrat, R. M., Dickens, B., **Atomic ordering in a 15-type phases in the vanadium-nickel and vanadium-cobalt systems,** *J. Appl. Phys.* **45,** No. 9, 3726-3728 (Sept. 1974).

Key words: A 15 phases; atomic ordering; magnetic structure; neutron diffraction; superconductivity; vanadium alloys.

Atomic ordering in the V-Ni and V-Co A 15-type phases has been studied using neutron diffraction. The V-Ni Structure is shown to be ordered to the maximum extent permitted by the "off stoichiometric" composition, $V_{77.5}Ni_{22.5}$. The V-Co structure possessing the "ideal" composition $V_{75.0}Co_{25.0}$ is also highly ordered. However, the V-Co diffraction data are less accurate due to neutron absorption by the cobalt atoms and interference from the sample holder. No magnetic structures were detected in the V-Co phase at 4.2 K.

Waxman, M., Davis, H. A., Hastings, J. R., **A new determination of the second virial coefficient of carbon dioxide at temperatures between 0 and 150 °C, and an evaluation of its reliability,** *Proc. Sixth Symp. on Thermophysical Properties, Atlanta, Ga., Aug. 6-10, 1973,* pp. 245-255 (Aug. 1973).

Key words: Burnett data reduction; carbon dioxide; nonlinear analysis; second virial coefficient.

Values of the second virial coefficient of carbon dioxide have been determined to an estimated reliability of 0.3 cm³/mole from Burnett PVT measurements taken over the pressure range from 2 to 35 bar at six temperatures between 0 and 150 °C. Our values, from −150 to −51 cm³/mole, compare favorably with those obtained from a recent correlation of literature values and are in substantial disagreement with the values previously determined from both the Burnett and the piezometer methods by Dadson and coworkers. The nonlinear least-squares analysis of Burnett data and our error analysis are discussed extensively and illustrated with results for carbon dioxide, helium, and ethylene. An algorithm, recently developed by M. Waxman, for the least-squares evaluation of parameters in nonlinear implicit equations, such as the Burnett pressure equation, is described.

Wiederhorn, S. M., Evans, A. G., Fuller, E. R., Johnson, H., **Application of fracture mechanics to space-shuttle windows,** *J. Amer. Ceram. Soc.* **57,** No. 7, 319-323 (July 1974).

Key words: fracture; glass; proof testing; static fatigue; stress corrosion.

The fracture properties of an ultralow-expansion glass intended for use in windows for the Space Shuttle were characterized by strength and fracture-mechanics techniques to provide reliable design data. Proof-test diagrams for predicting minimum times-to-failure under specified service loads were developed from measurements of subcritical crack growth in water and air. Failure predictions were confirmed from strength measurements in water. In vacuum ($< 10^{-4}$ torr), the fracture behavior was similar to that of other high-SiO_2 glasses, as evidenced by the absence of subcritical crack growth and by insensitivity of the critical stress intensity factor to temperature.

Wiederhorn, S. M., Johnson, H., Diness, A. M., Heuer, A. H., **Fracture of glass in vacuum,** *J. Amer. Ceram. Soc.* **57,** No. 8, 336-341 (Aug. 1974).

Key words: crack propagation; fracture; fracture mechanics; glass; strength.

The fracture of 6 glasses was studied in vacuum, $< 10^{-4}$ torr (10^{-2} N/m^2), as a function of temperature from 25 to 775 °C. Subcritical crack growth was observed in 4 of the glasses. Activation energies for crack motion ranged from 60 to 176 kcal/mol. The glasses which did not exhibit slow crack growth were "anomalous" glasses with abnormal thermal and elastic properties. Critical stress intensity factors for these 2 glasses increased ≈ 10 percent as the temperature increased to ≈ 600 °C. It is felt that subcritical crack growth is not the result of alkali-ion diffusion or viscous flow but rather of a thermally activated growth process which depends on the crack-tip structure in the glass. A narrow cohesive region at the crack tip favors subcritical crack growth, whereas a wide region favors abrupt fracture.

Wiese, W. L., Kelleher, D. E., **Asymmetries in Stark-broadened Balmer lines,** *Proc. 10th Int. Conf. on Phenomena in Ionized Gases, Oxford, England, Sept. 13-18, 1971,* p. 377 (1971).

Key words: assymmetries; hydrogen lines; line shifts; Stark-broadening.

Small asymmetries have been observed in the Stark-broadened hydrogen lines H_β and H_γ. They are most pronounced in the line wings, where the red wing is about 15 percent stronger than the blue one. Another asymmetry occurs between the two peaks of H_β where the blue peak is about 4 percent higher than the red one. For the central component of H_γ a small red shift is measured. The experimental results are compared with theoretical estimates and qualitative agreement is found. All experimental observations are made from a hydrogen plasma which is generated in a wall-stabilized arc.

Wiese, W. L., McClelland, J. F., Kelleher, D. E., Paquette, D. R., **Continuous emission from hydrogen plasmas. II. Experimental studies with a wall-stabilized arc,** *Proc. 9th Int. Conf. on Phenomena in Ionized Gases, Bucharest, Romania,* p. 596 (Sept. 1969).

Key words: continuum; emission intensity; hydrogen; plasma.

A wall-stabilized arc operating in hydrogen is used for the measurement of the continuous hydrogen emission in the visible and near ultraviolet regions of the spectrum. The arc plasma is spectroscopically analyzed, and measured continuum intensities are compared with recent extensive calculated values. Consistency is observed at all measured wavelengths.

Willis, P. M., Fox, M. R., **Computers for the inexperienced and impecunious,** *Liberal Education* **55,** No. 4, 545-550 (Dec. 1969).

Key words: computer science; computers; Hood College; research tool; time sharing; undergraduate education.

Hood College, a small liberal arts college in Frederick, Md., collaborated with the National Bureau of Standards in Gaithersburg in developing a work-study program in computing science that has served to introduce students and faculty to the capabilities and limitations of the digital computer. The program, sponsored by the National Science Foundation, resulted in four small liberal arts colleges establishing a computer appreciation course at nominal cost that has wide applicability to similar colleges which have access to and assistance in instruction from nearby government or industrial laboratories with computer capability. Details of the experiment along with costs are provided in sequence for the two years it encompassed.

Wilson, W. K., Parks, E. J., **Research program on stability of records at the National Bureau of Standards,** (Proc. 22nd TAPPI Testing Conference, Savannah, Ga., Oct. 7, 1971), *TAPPI* **55,** No. 1, 151-161 (1972).

Key words: accelerated aging; dry breaking load; paper; pH; records; reflectance; specifications; stability; wet breaking load.

An outline is given of historical origins and the current status of research into records preservation at the National Bureau of Standards. The principal effort concerns causes of the degradation of paper in storage. As many compositional and environmental variables contribute to the degradation of paper, it is not practical to analyze every potential variable. Some representative data are given from which it is concluded that (1) aging processes in dry and humid gases are mechanistically different; (2) increases in acidity are concurrent with decreases in the dry breaking load of paper, but not *functionally* related; (3) blue reflectance decreases as acidity increases and the dry breaking load decreases; (4) thermal analyis may be a crude but useful tool for detecting impermanence in paper. While an interim specification for permanence may be based on pH, it appears that an accelerated aging test must eventually be specified. The validity of dry oven aging is questionable.

Wilson, W. K., **Test methods for determining the effect of various treatments on paper,** *Proc. Int. Inst. for Conservation of Historic and Artistic Works (IIC) Congress, Lisbon, Portugal, Oct. 9-13, 1972,* pp. 985-994 (1972).

Key words: paper; paper test methods; restoration; restoration of paper; test methods for paper; treatment of paper.

Several methods are described that may be used in the evaluation of the effects of various restoration treatments on paper documents and works of art. References are given to standard methods and to other sources of information that would be of value to the restorer. The necessity for judging each situation as a separate entity is emphasized.

Wright, J., **Integration of the performance concept into building regulation,** *Proc. 3rd South African Symp. National Building Regulations, Durban, South Africa, May 17, 1974,* pp. 20-23 (1974).

Key words: building codes; building technology; energy conservation; evaluation and acceptance system; National Bureau of Standards; National Conference of States on Building Codes and Standards; performance concept.

Building regulation is an exercise of the police power and is therefore, by authority of the United States Constitution, a function of the member States of the Federal republic. But historically building has been a local enterprise and the States left its regulation to the cities since so many regulatory issues, e.g. conflagration, dealt with circumstances of urban life. The result is a mosaic of thousands of regulatory jurisdictions. This situation imposes burdens on building technology because each jurisdiction has its own set of standards (called a code) and enforcement practices. While traditional technology has managed to cope fairly well with the multiplicity of regulations and practices, innovative technology has been less successful. Performance standards would help to offset this imbalance since they are equally accommodating of new and traditional technology. However, performance standards require a performance evaluation and acceptance system if they are to be usefully promulgated. This is a key concept with the relatively new National Conference of States on Building Codes and Standards, an organization working to improve the regulatory climate. At the request of the Conference, the National Bureau of Standards (NBS) has prepared a document called "Draft Design and Evaluation Criteria for the Conservation of Energy in Buildings." The document is based on the performance concept with which NBS has had considerable experience. The NBS effort is also addressed to institutional mechanisms, including those necessary for a performance evaluation and acceptance system. The latter is seen as a complement to—not a competitor of—the established regulatory system.

Wright, J. R., Achenbach, P. R., Editors, **Energy Conservation in Buildings,** (Proc. Scientific American Roundtable of Energy Conservation in Buildings, New York, N.Y., Aug. 29, 1973), *Sci. Amer. Spec. Publ.*, 79 pages (1973).

Key words: buildings; conservation; energy; energy sources; measurement; simulation; thermal efficiency.

More base data is needed with respect to energy resources and us. Better measurement in terms of both techniques and values is suggested in the physical science aspects of energy and in our understanding of man and the energy-related attributes he requires of his shelter. Americans must stop wasting energy and at the same time develop new energy technologies. The roundtable offered numerous suggestions for the near-, mid- and long-range futures.

Wright, J. R., Herron, W. R., **Housing research at the National Bureau of Standards,** *Proc. Silver Jubilee Celebration of the Central Building Research Institute of India, Roorkee, India, Feb. 29-Mar. 2, 1973*, pp. 19-24 (1973).

Key words: building research; industrial building; performance criteria; total energy.

As the Central Building Research Institute at Roorkee is holding its Silver Jubilee, there is abroad in the world a great demand for relevance of many activities formerly left to random coordination. This is true in the United States of America and to some degree is the cry of all mankind. The Central Building Research Institute is to be commended for the achievement of relevance between the requirements of the people of India and their building research efforts. This has been accomplished by a steadfast adherence to the principle that sophisticated science can be turned to practical applications by research which recognizes the need to gear these applications into the patterns of everyday life in India. The thrust of this paper is to establish the realization that "Housing is a Social Process," since it involves a continuously changing interrelationship between national cultural goals, the designers, builders, and users. This realization is achieved to a varying degree from one culture to another. Some of the work described herein will show courses of action which can enhance the social significance of the building process.

Wright, J. R., Herron, W. R., **Response to "J. B. Dick Report,"** *Proc. 5th CIB Congress on Research into Practice. The Challenge of Application, Paris, France, June 1971*, pp. 275-279 (1971).

Key words: BREAKTHROUGH; building performance; construction; contracting; performance assessment; performance concept; performance products; performance testing; user needs.

This paper responds to a provocative paper prepared by Mr. J. B. Dick, Director, Building Research Station in England, for the 5th CIB Congress, June 22-30, 1971, at Versailles, France, entitled "Design Aids: Evaluation Methods for Buildings, Components and Materials." The intent of this paper is to defend the Performance Concept and its application to building construction. Such a defense must dispel misconceptions which have developed from the limited size of past demonstration projects based on this concept. If these false beliefs are not recognized, they could seriously limit future development and use of the performance concept.

Wright, J. R., Leyendecker, E. V., **Measuring the performance of industrialized housing under "Operation Breakthrough,"** *Proc. 5th CIB Congress on Research into Practice. The Challenge of Application, Paris, France, June 1971*, pp. 303-308 (1971).

Key words: certification; guide criteria; innovative housing; Operation BREAKTHROUGH; PERFORMANCE criteria; performance evaluation.

The National Bureau of Standards, Department of Commerce, is conducting the technical evaluation of "Operation BREAKTHROUGH" housing systems for the Department of Housing and Urban Development. This paper discussed the BREAKTHROUGH team's development of performance criteria and describes the philosophy used in developing the criteria. An example of how the criteria can be used in the evaluation process leading to certification is discussed.

Wright, R. N., **Buckling of plane or prismatic structures,** *Proc. RILEM Colloque Int. Symp., Buenos Aires, Argentina, Sept. 13-18, 1971*, pp. 1-13 (Instituto Nacional de Technologia Industrial, Buenos Aires, Argentina, 1971).

Key words: buckling; computers; experimental methods; instability; models; structures.

The papers in this topic address the purposes for experimental analysis of plane and prismatic structures. The report discusses papers dealing with the behavior of reinforced and prestressed concrete structures and metal structures. Within each category, local instability, member instability, and instability of assemblages are considered in the cited order. Finally, papers are discussed which treat aspects of experimental technology that are independent of the structural technology.

Wright, R. N., Yokel, F. Y., **A concept for limit states design,** *Proc. ASCE-IABSE Int. Conf., Bethlehem, Pa., Aug. 21-25, 1972, Conf. Preprints on Planning and Design of Tall Buildings*, **A**, 395-399 (1972).

Key words: design mode; limit states design; load; performance criteria; reinforced concrete; reliability; resistance mode; safety; serviceability; stability; structures.

The state-of-the-art reports presented in behalf of Committee 26 are summarized in this paper. Basic concepts and terminology associated with limit states design are discussed and a more general approach is suggested in which scheme-independent performance criteria would be used as a common basis for criteria for limit states design for all material applications. This approach would permit consistency among various material oriented design philosophies.

Wyckoff, J. M., Chilton, A. B., **Dose due to practical neutron energy distributions incident on concrete shielding walls,** *Proc. Third Int. Congress of the International Radiation Protection Association, Washington, D.C., Sept. 9-14, 1973*, pp. 694-699 (Feb. 1974).

Key words: concrete walls; neutron shielding; particle accelerators; rem.

In order to calculate the dose equivalent for persons on the far side of an ordinary concrete shielding wall from a plane parallel source of neutrons, published monoenergetic neutron data and practical neutron spectra have been folded together. Some interpolation of the monoenergetic neutron data, both in energy and slab thickness, was required to prepare the data for computation in steps of 50 g/cm². The result is a set of useful dose-equivalent data for walls as thick as 800 g/cm² used to shield particle accelerators producing neutrons up to 100 MeV in energy. A simple empirically derived, analytical expression for the dose equivalent for walls of 50 to 800 g/cm² thickness is given with suitable constants for neutron spectra produced by more than 60 selected examples of the following reactions: slow and fast neutron induced fission, (γ,n), (p,n), $(^3He,n)$, (α,n) and fission (γ,n).

Wyckoff, J. M., **Measurements for radiation safety,** *Proc. 19th Annual Meeting of the Institute of Environmental Sciences, Anaheim, Calif., Apr. 2-5, 1973*, pp. 130-135 (1973).

Key words: government agencies; measurement assurance program; permissible limits; radiation; regulations; standards; transfer standards.

Good measurements are the key to safe application of both ionizing and nonionizing radiation in industry, medicine and consumer products. The National Bureau of Standards, as the Nation's primary

source of physical measurement capability, is expanding its measurement services to radiation users. At the same time, it works closely with federal regulatory agencies such as AEC, BRH, NIOSH, and EPA to assist them in preparation of regulations containing realistic measurement requirements. The state of the measurement art in x-ray, nuclide, ultraviolet, laser, electromagnetic and ultrasonic radiation measurements will be reviewed highlighting the need for stable and accurate transfer standards to serve the safety community.

Wyckoff, J. M., Pruitt, J. S., Svensson, G., **Dose vs. angle and depth produced by 20 to 100 MeV electrons incident on thick targets,** (Proc. Int. Congress on Protection against Accelerator and Space Radiation, Cern, Geneva, Switzerland, Apr. 26-30, 1971), *Health Phys. CERN 71-16*, **2**, 773-797 (July 1, 1971).

Key words: electrons; MeV electrons; targets; thick targets.

When energetic electrons strike a thick target a number of processes lead to photons, electrons and neutrons leaving that target. The dose produced by this emerging radiation has been measured as a function of angle and depth in a polymethylmethacrylate phantom for incident 20 to 100 MeV electrons. While this is a special geometry, it is fairly typical and the general nature of the distribution may be of interest in planning of exposure and shielding against exposure. The measurement technique, involving the use of a large number of small thermoluminescent dosimeters, is shown to produce results that compare very favorably with recent calculations made for the particular 30 MeV electron target conditions.

Wyly, R. S., Orloski, M. J., **Studies of reduced-size venting of sanitary drainage systems in the USA,** (Proc. CIB Commission W62 Symp. on Gravity Drainage, Stockholm, Sweden, Sept. 24-25, 1973), Paper 13 in *Drainage Services in Buildings, D14:1973*, pp. 13:1–13:19 (National Swedish Building Research, Stockholm, Sweden, 1973).

Key words: air demand; criteria for venting; reduced-size venting; trap performance; trap-seal retention/reduction; venting criteria; venting, reduced-size.

Results of experimental studies of reduced-size venting in the USA are summarized, tentative criteria are presented, and the need for further work leading to a general method for computation of vent sizes is discussed. Experimentation with vents smaller than customarily allowed has shown satisfactory performance under selected conditions that seem representative of the service environment.

Among the significant findings were: (1) trap-seal retention was adequate with peak fluctuating suction of as much as 75 mm water column for a water closet trap, and about 38 mm for a lavatory P-trap, compared with the 25 mm presently assumed for design, (2) air demand rates required to assure adequate trap-seal retention were significantly less than presently assumed, probably because of effective "slippage" between air and water in short stacks and because of air circulation in systems comprised of a piping "network," (3) discharge profile and accumulative duration of test loading significantly affected idle trap-seal performance, and (4) back pressure (blow-back) was a significant criterion for system performance, particularly at the ground-floor elevation of a high-rise system.

Yakowitz, H., **A practical examination of the Kossel x-ray diffraction technique,** Chapter 11 in *Microprobe Analysis*, C. A. Andersen, Ed., pp. 383-421 (John Wiley & Sons, Inc., New York, N.Y., 1973).

Key words: crystal orientation; error propagation; Kossel lines; lattice spacings; stress-strain maps; x-ray diffraction.

The divergent beam (Kossel) x-ray diffraction method can provide lattice spacing data and crystallographic orientation information from regions 15 μm in diameter by 2 to 10,000 μm in depth depending on the experimental conditions and the target. A typical depth value is 50 to 75 μm. In addition, all of the (hkl) planes of a family are separated, i.e., if (222) appears then (222) will appear as a separate entity. This last circumstance permits a Kossel Internal Stress-Strain (KISS) analysis to be carried out in a straightforward way. In particular, the Cauchy strains, principal strains and their axes, principal stresses and their axes, maximum shear strain in any (hkl) plane and the total stored elastic energy in the irradiated region can be calcuated for lightly strained materials. This paper will describe the Kossel method in general with emphasis on the KISS analysis—especially from the point of view of reliability of the KISS results. The object will be to illustrate the power of the KISS but also to point out its limitations in practice. Experimental design will be discussed in terms of its effect on the stress-strain analysis results.

Yakowitz, H., Fiori, C. E., Newbury, D. E., **Implications of specimen current and time differentiated imaging in scanning electron microscopy,** (Proc. Sixth Annual Scanning Electron Microscopy Symp., Chicago, Ill., Apr. 21-23, 1973), Chapter in *Scanning Electron Microscopy/1973, Part I*, pp. 173-180 (IIT Research Institute, Chicago, Ill., Apr. 1973).

Key words: channelling patterns; iron; lunar samples; magnetic contrast; scanning electron microscope; signal differentiation; specimen current images.

The technique of specimen current imaging has not been widely used in the SEM field, primarily because of a lack of an adequate amplifier system to operate with the low beam current, typically 5×10^{-11} amperes, used in high resolution work. A current amplifier capable of providing images of the specimen current signal when that signal is as low as 5×10^{-12} amperes is described briefly. This instrument also provides differentiation with respect to time (time differentiation) of either the absorbed current or secondary electron signals from the specimen.

Micrographs comparing the secondary electron and specimen current images under various operating conditions are discussed in terms of picture quality. Often, the specimen current image provides information which cannot be obtained from the emissive mode (primary or secondary electrons) image or else is especially difficult to obtain because of specimen/collector geometry. In the past, direct current amplifiers were unable to operate with sufficiently low specimen currents for high resolution photography. Therefore, the impression that specimen current imaging was intrinsically inferior to secondary electron imaging was promulgated. The use of present day equipment indicates that this impression is not correct.

The extra flexibility added by a time differentiating device for both the secondary electron and specimen current modes is described. Mixing the normal signal with the time differentiated signal in all proportions is desirable in order to retain some field depth while reducing gray level disparity.

Yeh, K-N., Birky, M. M., Huggett, C., **Calorimetric study of flammable fabrics. II. Analysis of flame retardant-treated cotton,** *J. Appl. Polym. Sci.* **17**, 255-268 (1973).

Key words: calorimetric; cellulose; flammability; flame retardant; heat; phosphorus; rate.

Efficiencies of three flame retardants for cellulose; phosphoric acid, diammonium phosphate and THPOH ammonia finish, have been evaluated based on the heat-release value and the rate of heat-release of treated fabrics burning in air measured with the isoperibol calorimeter. The results were compared and correlated with those obtained previously with the bomb calorimetric technique. Complete heat balances were obtained for the systems studied by correlation of the calorimetric data and the measurement of combustible gases evolved from the fabric burning in air. The rate of heat-release was found to correlate with 45° flame propagation rate. The results from the heat, rate and combustible gas measurements were interpretable in terms of existing mechanisms of flame retardant action.

Yonemura, G. T., **Image quality criterion for the identification of faces,** *LESP-RPT-0303.00,* 24 pages (U.S. Department of Justice, Law Enforcement Assistance Administration, National Institute of Law Enforcement and Criminal Justice, Washington, D.C., May 1974).

Key words: acutance; facial identification; identification in photographs; image quality; modulation transfer function.

This report describes an experiment, the resulting data, and recommendations concerning an image quality criterion for identification of faces in a photograph. It relates the psychological levels of visual performance to performance of photographic equipment in terms of acutance and modulation transfer function.

Yonemura, G. T., **Opponent-color-theory treatment of the CIE 1960 (u,v) diagram: Chromaticness difference and constant-hue loci,** *J. Opt. Soc. Amer.* **60,** No. 10, 1407-1409 (Oct. 1970).

Key words: chromaticity diagram; color difference; color hue; color theory.

An angular interpretation of the CIE 1960 (u,v) system is presented. This new development of the CIE 1964 (u,v) (U^*, V^*, W^*) system results in improved chromaticness-difference predictions and is more in accord with empirical constant-hue loci than the U^*, V^*, W^* system.

Young, R. H., Brewer, D., Kayser, R., Martin, R., Feriozi, D., Keller, R. A., **On the mechanism of quenching by amines: A new method for investigation of interactions with triplet states,** *Can. J. Chem.* **52,** No. 16, 2889-2893 (1974).

Key words: lasers; $^1\Delta O_2$; photochemistry.

Rate constants for the quenching of singlet oxygen by a series of substituted *N,N*-dimethylanilines were obtained by a direct method employing a dye-laser. The Hammett ρ value obtained from the data (− 1.71) suggests that a (partial) charge-transfer complex may be responsible for the quenching action. This rate data was combined with that obtained for the total quenching action on the sensitized photooxidation of 1,3-diphenylfuran. The quenching action on the photooxidation reaction is due to both the quenching of singlet oxygen and the quenching of the triplet state of the sensitizer (rose bengal or methylene blue). The combination of the data from each series of experiments resulted in rate constants of quenching of the triplet states of the sensitizers. A number of the *N,N*-dimethylanilines quenches the triplet states at the diffusion limit. Hammett ρ values (− 1.86 for rose bengal and − 4.19 for methylene blue) indicate that charge-transfer intermediates are probably responsible for the quenching action. This was confirmed by the observation of a transient intermediate assigned to the charge-transfer radical of methylene blue. The technique used here represents a novel approach to the investigation of triplet states.

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